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Finite element calculation of the interaction energy of shape memory alloy

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Key Words : Shape memory alloy (), Phase transformation(), Interaction energy (), Finite element analysis ()

Abstract

Strain energy due to the mechanical interaction between self-accommodation groups of martensitic phase transformation is called interaction energy. Evaluation of the interaction energy should be accurate since the energy appears in constitutive models for predicting the mechanical behavior of shape memory alloy. In this paper, the interaction energy is evaluated in terms of theoretical formulation and explicit finite element calculation. A simple example with two habit plane variants was considered. It was shown that the theoretical formulation assuming elastic interaction between the self-accommodation group and matrix gives larger interaction energy than explicit finite element calculation in which transformation softening is accounted for.

α_0 : reference strain rate (incompatibility) 가 . Huang

η_α : order parameter of α -th habit plane variant Brinson (2)

τ_α : critical resolved shear stress of α -th habit plane variant (interaction energy) (matrix) 가 가

γ_c : strain of fully transformed state 가 가 가 가 .

1. (phase transformation) (habit plane variant) (self accommodation group) .(1) 가 (softening)

† 가 2 가

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2.

Huang Brinson (2)

Fig. 1

(homogeneous)

(local)

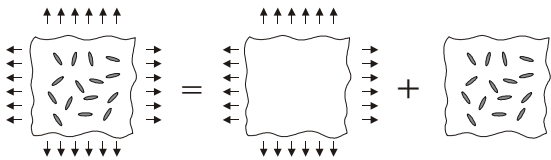
(global)

$$\begin{aligned} \sigma_{ij}^I &= \Sigma_{ij}^I = \Sigma_{ij} \\ \varepsilon_{ij}^I &= E_{ij}^I = E_{ij}^e \end{aligned}$$

(II)

0

I II



$$\begin{aligned} \Sigma_{ij} & & \Sigma_{ij}^I &= \Sigma_{ij} & \Sigma_{ij}^{II} &= 0 \\ E_{ij} &= E_{ij}^e + E_{ij}^p & E_{ij}^I &= E_{ij}^e & E_{ij}^{II} &= E_{ij}^p \\ \sigma_{ij} & & \sigma_{ij}^I &= \Sigma_{ij}^I & \sigma_{ij}^{II} & \\ \varepsilon_{ij} &= \varepsilon_{ij}^e + \varepsilon_{ij}^p & \varepsilon_{ij}^I &= E_{ij}^I & \varepsilon_{ij}^{II} &= \varepsilon_{ij}^{IIe} + \varepsilon_{ij}^{IIp} \end{aligned}$$

Fig. 1 Decomposition of total problem.

I II

$$\begin{aligned} \Sigma &= \Sigma^I \\ E &= E^e + E^p \\ \sigma &= \sigma^I + \sigma^{II} = \Sigma + \sigma^{II} \end{aligned}$$

$\varepsilon = \varepsilon^I + \varepsilon^{II} = E^e + \varepsilon^{IIe} + \varepsilon^{IIp}$
(elastic strain energy density)

$$W_{el} = \frac{1}{2V} \int_V \sigma_{ij} \varepsilon_{ij}^e dV$$

$$\begin{aligned} W_{el} &= \frac{1}{2V} \int_V (\Sigma_{ij} + \sigma_{ij}^{II}) (E_{ij}^e + \varepsilon_{ij}^{IIe}) dV \\ &= \frac{1}{2V} \int_V (\Sigma_{ij} + \sigma_{ij}^{II}) (E_{ij}^e + \varepsilon_{ij}^{II} - \varepsilon_{ij}^{IIp}) dV \\ &= \frac{1}{2V} \int_V \Sigma_{ij} E_{ij}^e dV - \frac{1}{2V} \int_V \sigma_{ij}^{II} \varepsilon_{ij}^{IIp} dV \\ &\quad + \frac{1}{2V} \int_V \Sigma_{ij} \varepsilon_{ij}^{IIe} dV + \frac{1}{2V} \int_V \sigma_{ij}^{II} (E_{ij}^e + \varepsilon_{ij}^{II}) dV \\ &\quad \int_V \Sigma_{ij} \varepsilon_{ij}^{IIe} dV = \Sigma_{ij} \int_V \varepsilon_{ij}^{IIe} dV = 0 \end{aligned}$$

$$\begin{aligned} &\int_V \sigma_{ij}^{II} (E_{ij}^e + \varepsilon_{ij}^{II}) dV \\ &= \int_V \sigma_{ij}^{II} E_{ij}^e dV + \int_V \sigma_{ij}^{II} \varepsilon_{ij}^{II} dV \\ &= 0 + \int_{\partial V} \sigma_{ij}^{II} n_j u_i^{II} dV - \int_V \sigma_{ij,j}^{II} u_i^{II} dV \\ &= 0 \end{aligned}$$

II

traction 0

$$W_{el} = \frac{1}{2} \Sigma_{ij} E_{ij}^e - \frac{1}{2V} \int_V \sigma_{ij}^{II} \varepsilon_{ij}^{IIp} dV$$

가

(interaction energy)

$$W_{int} = -\frac{1}{2V} \int_V \sigma_{ij}^{II} \varepsilon_{ij}^{IIp} dV \quad (1)$$

(self accommodation group)

가

가

N plane variant)

가

, V

(habit

G

$$, N = G \times V \quad . \alpha$$

$$\eta_\alpha \quad , \alpha \text{ 가 } k$$

$$, \bar{\eta}_k,$$

$$\bar{\eta}_k = \sum_{\alpha=1}^V \eta_\alpha$$

. α

$$\varepsilon_{ij}^\alpha$$

$$\varepsilon_{ij}^\alpha = \frac{1}{2} \gamma_c (m_i^\alpha n_j^\alpha + n_i^\alpha m_j^\alpha)$$

$$\gamma_c \quad , m_i^\alpha, n_i^\alpha$$

(habit plane)

. k

$$\bar{\varepsilon}_{ij}^k,$$

$$\bar{\varepsilon}_{ij}^k = \frac{1}{V_k} \int_{V_k} \varepsilon_{ij}^\alpha dV$$

$$= \frac{1}{V_k} (\varepsilon_{ij}^1 v^1 + \varepsilon_{ij}^2 v^2 + \dots + \varepsilon_{ij}^V v^V)$$

$$= \frac{1}{\bar{\eta}_k} \sum_{\alpha=1}^V \eta_\alpha \varepsilon_{ij}^\alpha$$

$$V_k \quad v^\alpha \quad k \quad \alpha$$

, (microscopically) v^α

$$\varepsilon_{ij}^{lp} = 0 \quad \bar{\eta}_k = V_k / V \quad . k$$

$$\langle \sigma_{ij} \rangle_k \quad \bar{\sigma}_{ij}^k$$

$$\sigma_{ij}^{ll} = \langle \sigma_{ij}^{ll} \rangle + \delta \sigma_{ij}^{ll}$$

(1)

$$W_{\text{int}} = -\frac{1}{2V} \int_V \sigma_{ij}^{ll} \varepsilon_{ij}^{lp} dV$$

$$= -\frac{1}{2V} \sum_{k=1}^G \int_{V_k} \sigma_{ij}^{ll} \varepsilon_{ij}^{lp} dV$$

$$= -\frac{1}{2V} \sum_{k=1}^G \int_{V_k} (\langle \sigma_{ij}^{ll} \rangle + \delta \sigma_{ij}^{ll}) (\langle \varepsilon_{ij}^{lp} \rangle + \delta \varepsilon_{ij}^{lp}) dV$$

$$\approx -\frac{1}{2V} \sum_{k=1}^G \int_{V_k} \langle \sigma_{ij}^{ll} \rangle \langle \varepsilon_{ij}^{lp} \rangle dV$$

$$= -\frac{1}{2V} \sum_{k=1}^G \langle \sigma_{ij}^{ll} \rangle_k \langle \varepsilon_{ij}^{lp} \rangle_k V_k$$

$$= -\frac{1}{2} \sum_{k=1}^G \bar{\sigma}_{ij}^k \bar{\varepsilon}_{ij}^k \bar{\eta}_k$$

Eshelby

0

(inclusion)

$$\bar{\sigma}_{ij}^k = C_{ijmn} (S_{mnpq} - I_{mnpq}) (\bar{\varepsilon}_{pq}^k - E_{pq}^{ll})$$

$$= \hat{\sigma}_{ij}^k - C_{ijmn} (S_{mnpq} - I_{mnpq}) \sum_{l=1}^G \bar{\eta}_l \bar{\varepsilon}_{pq}^l$$

$$= \hat{\sigma}_{ij}^k - \sum_{l=1}^G \bar{\eta}_l \hat{\sigma}_{ij}^l$$

$$, \hat{\sigma}_{ij}^k = C_{ijmn} (S_{mnpq} - I_{mnpq}) \bar{\varepsilon}_{pq}^k$$

(summation convention)

 S_{ijkl} Eshelby

$$W_{\text{int}} = -\frac{1}{2} \sum_{k=1}^G \bar{\sigma}_{ij}^k \bar{\varepsilon}_{ij}^k \bar{\eta}_k$$

$$= -\frac{1}{2} \sum_{k=1}^G \left(\hat{\sigma}_{ij}^k - \sum_{l=1}^G \bar{\eta}_l \hat{\sigma}_{ij}^l \right) \bar{\varepsilon}_{ij}^k \bar{\eta}_k$$

(2)

3.

(Gibbs free energy) Φ (complementary free energy) Ψ

(2)

$$\Psi(\Sigma, T, \eta_\alpha) = -(\Phi(\Sigma, T, \eta_\alpha) - \sum_{ij} E_{ij})$$

가

(dissipative

energy)

$$d\Psi|_{\Sigma, T} = dW_d$$

(3)

$$W_d = \sum_{\alpha=1}^N \left(\int_S \beta \dot{\eta}_\alpha d\eta_\alpha \right)$$

(4)

 β

(3) (4)

S η_α

$$\begin{aligned} \beta \dot{\eta}_\alpha &= -\frac{\partial \Phi}{\partial \eta_\alpha} + \Sigma_{ij} \epsilon_{ij}^\alpha \\ &= -\frac{\partial W_{chem}^\alpha}{\partial \eta_\alpha} - \frac{\partial W_{el}}{\partial \eta_\alpha} + \Sigma_{ij} \epsilon_{ij}^\alpha \\ &= -\tau_c \gamma_c - \frac{\partial W_{int}}{\partial \eta_\alpha} + \tau_\alpha \gamma_c \\ &= \gamma_c (\tau_\alpha - \tau_c) - \frac{\partial W_{int}}{\partial \eta_\alpha} \end{aligned}$$

$$\dot{\gamma}_\alpha = a_0 \left\{ \gamma_c (\tau_\alpha - \tau_c) - \frac{\partial W_{int}}{\partial \eta_\alpha} \right\} \quad (5)$$

$$W_{chem}^\alpha = \eta_\alpha \tau_c \gamma_c, \quad \gamma_\alpha = \eta_\alpha \gamma_c,$$

$$\tau_\alpha = \Sigma_{ij} m_i^\alpha n_j^\alpha$$

(resolved shear stress) . (5)

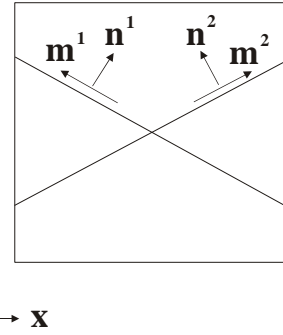


Fig. 2 Two transformation systems. In this model volumetric component of transformation strain is assumed zero.

Table 1 Material parameters

Young's modulus	47.9 GPa
Poisson's ratio	0.46
γ_c	0.13
τ_c	15 MPa
a_0	$0.001 \text{ Pa}^{-1} \text{ sec}^{-1}$
N	2

(5)

4.

가

(1),

NiTi
가

Fig. 2
m

$$\begin{aligned} \mathbf{n}^1 &= \left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0 \right), \quad \mathbf{n}^2 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0 \right) \\ \mathbf{m}^1 &= \left(-\frac{\sqrt{3}}{2}, \frac{1}{2}, 0 \right), \quad \mathbf{m}^2 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}, 0 \right) \end{aligned}$$

0.01m x 0.01m x 0.01m

1

가 , $\dot{E}_{yy} = 2000 \text{ (1/s)}$

가 . 2

N=2

G 1 2 가 가 . G=1

V 1 . G=1 V 2 , G=2

$\eta_1 \eta_2$

(2)

n

가
Table 1

Fig. 3

(1 group)

(2 groups)
가

0.01m x 0.01m x 0.01m 64
 가 , 2
 가 1
 가 2 Fig.4
 가
 (matrix) (inclusion)
 (solution)

$$\sigma_{ij}^{II} \quad (1)$$

$$\varepsilon_{ij}^{IIp} = \sum_{\alpha=1}^v \eta_{\alpha} \varepsilon_{ij}^{\alpha} \quad (2)$$

$$\Sigma_{22} = 0 \quad \varepsilon_{ij}^{IIp} \quad (2)$$

$$\sum_{\alpha=1}^v \eta_{\alpha} \varepsilon_{ij}^{\alpha} \quad \text{가}$$

가 Fig. 3
 가
 , 2
 (2)

Fig. 5
 group 2 groups)
 1 가 (1
 (finite element)
 1 가

Fig. 6
 가
 가
 가
 ε_{yy} 가 0.075
 가

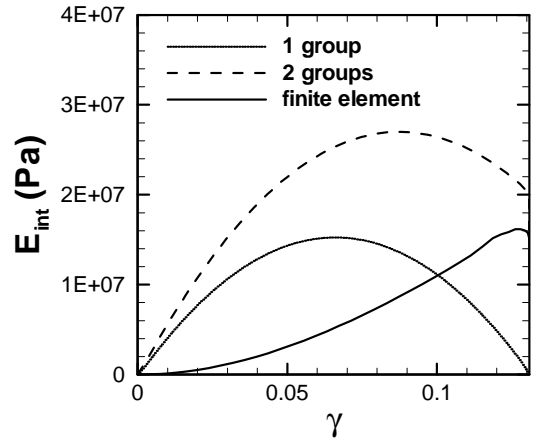


Fig. 3 Interaction energy. $\gamma = \gamma_1 + \gamma_2$ for 1 group or 2 groups, and $\gamma = \gamma_1$ for finite element. For 1 group, two habit plane variants belong to one self accommodation group. For 2 groups, only one habit plane variant belongs to one group. For finite element, self accommodation groups are modeled by finite elements.

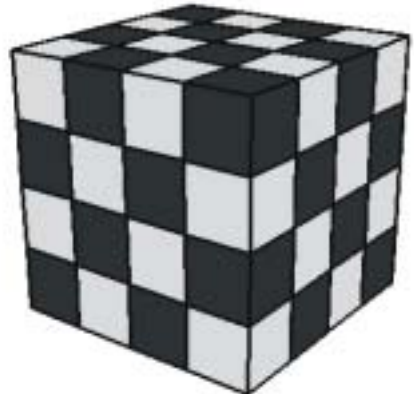


Fig. 4 Finite element model of self accommodation groups. Dark and light regions correspond to two self accommodation groups.

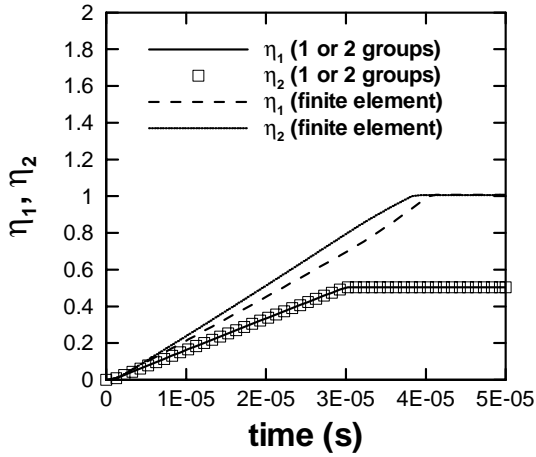


Fig. 5 Volume fraction of each habit plane variant with respect to time.

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- (2) Huang, M.S. and Brinson, L.C., 1998, A multivariant model for single crystal shape memory alloy behavior, *J. Mech. Phys. Solids* V46, pp. 1379-1409.

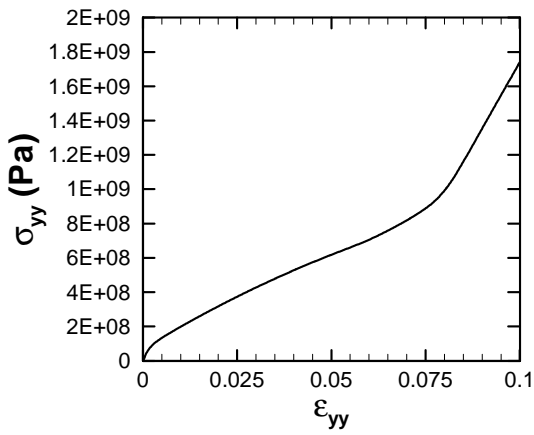


Fig. 6 Average tensile stress vs. strain in explicit finite element modeling of self accommodation groups.

5.

가
가

(self-consistent)
가