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Constitutive modeling of functionally graded material and its application to fracture in FGM

M. Nakagi, Y. Wu, Y. Shibata, S. Hagihara
Department of Mechanical Systems Engineering, Kyushu Institute of Technology, Iizuka-City, Japan

Abstract
An analytical methodology is shown for studying a crack in a functionally graded material subjected to an intense thermal shock load. A theoretical elastoplastic material modeling of the functionally graded material is presented. Also independently a computational procedure of an elastoplastic constitutive law is introduced with the use of a micromechanics analysis and a hierarchical neural network algorithm. The material is composed of ZrO_2 and $Ti-6Al-4V$, where the plastic flow is considered to occur in the titanium alloy phase. To detect the crack-tip fracture severity in the highly inhomogeneous media, T^*integral parameter is employed for the thermal shock problem of the cracked material.

Introduction
In high temperature technology, multi-material bodies comprised of ceramics and high toughness materials such as metals have been thought. The discrepancies in the thermal expansion rates and other material properties between the materials causes a strength problems at the interface. Functionally graded material(FGM) is, hence, devised in the manner that the material composition is continuously varied with location in order to remove the strain discontinuity. By properly grading the composition of the constituents, the thermal stresses in the FGM may be minimized. FGM is, thus, inherently inhomogeneous, and in addition thermally inhomogeneous such that the material properties change over the wide range of temperature to that the material is designated to be subjected.

The FGM is still on the materials research and development stage. To design the material, the prompt establishment of the analytical methodology is urged. For the analysis of such a material behavior and the structure, rapidly developing computational mechanics is best suited for its complexity. In the computational analysis of the FGM, the local macroscopic constitutive law for the averaged medium, where the matrix and/or the inclusion phases undergo thermo-elastoplasticity, must be known. When plastic flow occurs, if the volume fraction of the inclusion phase is high, interactions between inclusions may give a significant effect on the overall stress-strain response.

Although the inclusion size is several order greater than that of FGM, particle reinforced composites have the analogous constituency to the FGM. Tandon and Weng[1] introduced the concept of particle reinforced plasticity with the use of secant moduli method based on the deformation theory of plasticity. Tohgo and Weng[2] extended their work with the tangent modulus method. Their composite theory, as most of other investigators in the composite area did, is based on the Eshelby's equivalent inclusion theory[3] and the mean field concept by Mori and Tanaka[4]. Since the methods are valid only under a proportional loading, the constitutive law is not applicable to the plastic composites when the history dependent deformation is not negligible.

Due to the limitations that the available analytical models have, the general elastoplastic constitutive law for the plastic composites of the class is not yet fully established. Moreover, none of the models can, with a sufficient accuracy, account for the complicated plastic effects with the inclusion, the interaction, and the possible damage of or between the constituent phases.

In the present paper, a fracture of the functionally graded material under intense thermal shock, where a material phase will be subjected to the plastic deformation in high temperature, is addressed. The FGM is consisted of two material phases, which are a ceramic, ZrO_2, and a titanium alloy, $Ti-6Al-4V$. For the problem, a finite element analysis of micromechanics model, a development of an incremental constitutive relation based on the Eshelby's equivalent inclusion method and the Mori-Tanaka's mean field concept, and a generalization with a neural network were performed.

(1) Micromechanics analysis of FGM with spherical grain model

It is no doubt that the most reliable constitutive behavior of the FGM may be obtained from an experiment. Due to the lack of such in the present, a numerical micromechanics analysis by FEM is performed to

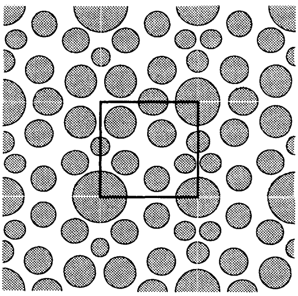


Figure 1. FGM grain model and reference domain.

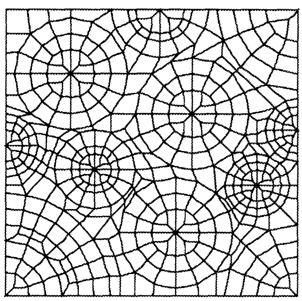


Figure 2. Finite element modeling of reference domain.

substitutes the experiment. To estimate the overall tensile stress-strain characteristics of the FGM composite, a reference volume of the two phase medium is analyzed. The matrix is represented by the ceramic, whereas the inclusion by the titanium alloy, in only which the plasticity is assumed to occur. The boundaries of the reference domain are subjected to symmetric boundary conditions, antisymmetric boundary condition, penalty constraints, or specified displacement constraint conditions depending on the uniaxial loading directions considered in the infinite body. The antisymmetric constraints make the ±45° tension possible with respect to the axes.

Even if the reference domain configuration is carefully arranged to bring a random distribution pattern in the composite model, still there remains a question of macroscopic anisotropy due to the stress interactions between particles caused by the periodicity of the reference domain. Hence, the results of the present domain are compared with two extreme cases of the particle distributed composite in the periodic square array of the uniformly sized inclusions; one case the loading is in line with the direction of the periodicity, and the other in the direction of 45° to the former. The periodic square array showed a conspicuous loading direction sensitivity especially in the plastic range. Whereas, the present reference volume exhibits the almost nil sensitivity. Which means that the present reference volume model may represent a random domain with a reasonable accuracy.

(2) **Incremental constitutive equation for FGM**

Independent from the aforementioned micromechanics constitutive investigation, derivation of a closed form incremental constitutive relation is attempted for the composite with the spherical inclusions. Eshelby's equivalent inclusion theory with an eigen strain is used to describe the average stress in the single inclusion phase. Mori-Tanaka's mean field theory is employed to generalize the above for the domain with many inclusions.

Consider an equivalent composite where the inclusion phase is replaced by an equivalent inclusion with the material same as that of the matrix. Denoting the matrix by subscript 1 and the inclusion by 2, whereas the script *s* represents the equivalent of the latter. Thus the equivalence is described by

$$d\underset{\sim}{\sigma}^{s} = d\underset{\sim}{\sigma}_{2}, \quad d\underset{\sim}{\varepsilon}_{s} = d\underset{\sim}{\varepsilon}_{2} \qquad (1)$$

Assume the strain in the inclusion phase can be decomposed such that:

$$d\underset{\sim}{\varepsilon}_{s} = d\underset{\sim}{\varepsilon}_{s}^{e} + d\underset{\sim}{\varepsilon}_{s}^{p} + d\underset{\sim}{\varepsilon}^{*} \qquad (2)$$

where $\underset{\sim}{\varepsilon}^{*}$ is the eigen strain. The elastic strain is written as,

$$d\underset{\sim}{\varepsilon}_{s}^{e} = \underset{\sim}{E}_{1}^{-1} : d\underset{\sim}{\sigma}_{2} \qquad (3)$$

The scheme in the present resumes that the eigen strain adjusts the stress in the equivalent phase in the elastic fashion while the total strain is kept

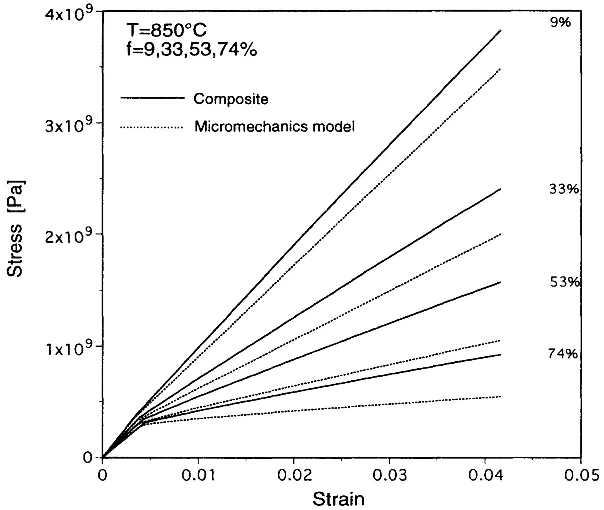


Figure 3. Stress-strain relations of composite with spherical inclusions.

identical to that of the real system.

The strain in single equivalent spherical inclusion in an infinite medium is given with the use of Eshelby tensor $\underset{\sim}{S}$ [3] by

$$d\underset{\sim}{\varepsilon}_s = d\underset{\sim}{\varepsilon}_1 + \underset{\sim}{S} : d\underset{\sim}{\varepsilon}^* \tag{4}$$

From Eq.2, the eigen strain will be

$$d\underset{\sim}{\varepsilon}^* = \left(\underset{\sim}{D}_2^{-1} - \underset{\sim}{E}_1^{-1}\right) : d\underset{\sim}{\sigma}^s - \left(\underset{\sim}{D}_1^{-1} - \underset{\sim}{E}_1^{-1}\right) : d\underset{\sim}{\sigma}_1 \tag{5}$$

In the above, $\underset{\sim}{E}$ and $\underset{\sim}{D}$ denote respectively the elastic and elastoplastic material tensors. When a number of inclusions are randomly distributed in the medium, Mori-Tanaka theory[4] can then be employed to describe the stresses in the equivalent phases for the external loading of $\underset{\sim}{\sigma}^0$, such that:

$$d\underset{\sim}{\sigma}_1 = d\underset{\sim}{\sigma}^0 - f\, d\underset{\sim}{\sigma}' \tag{6}$$

$$d\underset{\sim}{\sigma}^s = d\underset{\sim}{\sigma}^0 + (1 - f) d\underset{\sim}{\sigma}' \tag{7}$$

where, f is the volume fraction for the inclusion, and $d\underset{\sim}{\sigma}'$ denotes the stress discrepancy between the matrix and the inclusion. According to Eshelby,

$$d\underset{\sim}{\sigma}' = \underset{\sim}{E}^0 : d\underset{\sim}{\varepsilon}^* \tag{8}$$

$$\underset{\sim}{E}^0 = \underset{\sim}{E}_1 : \left(\underset{\sim}{S} - \underset{\sim}{I}\right) \tag{9}$$

Eqs.6 - 9 are used with Eq.5 to solve for the eigen strain to obtain,

$$d\underset{\sim}{\varepsilon}^* = \underset{\sim}{A}^* : d\underset{\sim}{\sigma}^0 \tag{10}$$

where,

$$\tilde{A}^{*} = \{\tilde{I} - [(1-f)\tilde{D}_{s}^{-1} + f\tilde{D}_{m}^{-1} - \tilde{E}_{1}^{-1}]:\tilde{E}^{0}\}^{-1}:(\tilde{D}_{s}^{-1} - \tilde{D}_{m}^{-1}) \quad (11)$$

Using the Mori-Tanaka theory for strain averaging, the average strain is written by

$$d\tilde{\bar{\varepsilon}} = \tilde{D}_{1}^{-1}:d\tilde{\sigma}^{0} + f\tilde{A}^{*}:d\tilde{\sigma}^{0} \quad (12)$$

Thus the incremental constitutive law for the average composite will be described such that:

$$d\tilde{\sigma}^{0} = (\tilde{D}_{1}^{-1} + f\tilde{A}^{*})^{-1}:d\tilde{\bar{\varepsilon}} \quad (13)$$

The constitutive relation is applicable for the case that the matrix and the inclusion phases undergo elastic or elastoplastic deformations.

The tensile test for the present constitutive law is performed, and compared with the micromechanics analysis by FEM mentioned in the previous section. The results are shown in Figure 3 for the various volume fractions. Considerable discrepancies are seen between the two results at the plastic stage for the high volume fractions. The underlying theory assumes that the volume fraction of inclusion is so small that there is no interaction between inclusions. Whereas, the micromechanics analysis precisely reflects the interaction.

(3) **Neural network application to constitutive relation of FGM**

As discussed in the above, the constitutive law, which does not account for the plastic interaction between inclusions, has the significant errors at high volume fractions. The most unambiguous way is to recruit the result of the micromechanics model itself for the constitutive relation in the FGM analysis. However, it is impossible to prepare vast data of arbitrary volume fractions and temperatures. Thus, the present effort was directed toward establishing a neural network procedure for the FGM constitutive law with the limited number of micromechanics analysis data. One of the powerful points of the neural network is that one can extend the number of degree of freedom of the system just by adding neurons without paying much attentions to the behavior of the data.

For the 6 volume fractions and 7 temperatures, the micromechanics

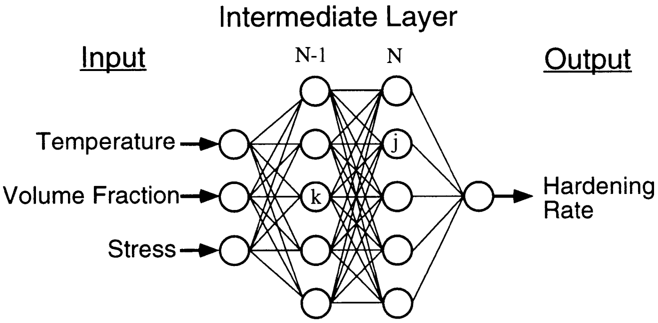


Figure 4. Hierarchical neural network

analysis for the pattern shown in Figure 1 were performed to serve as the teach data for a hierarchical neural network algorithm, which develops mapping between the plastic hardening rate of the FGM and the state variables that are stress, volume fraction, and temperature.

Volume Fraction(V)	0, 26, 42, 66, 90, 100	%
Temperature(T)	700, 750, 800, 850, 900, 950, 1000	℃

Denoting a state value that the neuron N_j^N has u_j^N, let the output from the neuron be:

$$v_j^N = f(u_j^N) \tag{14}$$

where the Sigmoid function

$$f(u) = \frac{1}{1+\exp(-u/t)} \tag{15}$$

which takes a value between 0 and 1 was used. Thus calculated output results are compared with the teach data. The weights at each neuron are subsequently modified by back propagation so that the total sum of the square of the error is minimized. The corrections to the weight and the threshold are given by,

$$\Delta W_{jk}^{N,N-1} = \Delta v_j^N f'(u_j^N) v_k^{N-1} \tag{16}$$

$$\Delta h_j^N = -\Delta v_j^N f'(u_j^N) \tag{17}$$

The modified weight and the threshold are respectively shown to be

$$W_{jk}^N = W_{jk}^N - (\eta \Delta W_{jk}^N + \alpha \Delta W'^N_{jk}) \tag{18}$$

$$h_j^N = h_j^N - (\eta \Delta h_j^N - \alpha \Delta h'^N_j) \tag{19}$$

where, η and α are computational constants. In the present, $\eta = 0.25$ and

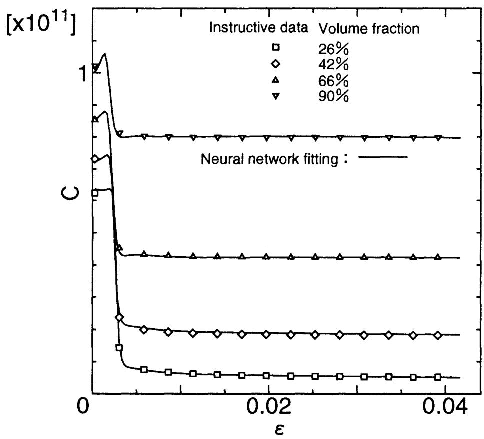


Figure 5. Fitted slope of stress-strain for spherical grain model.

α=0.9 , which provided with the best convergence are used.

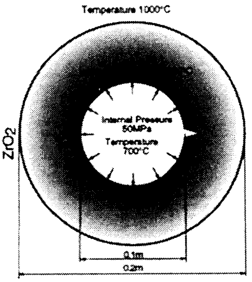
The process is repeated for approximately 40,000 times until the error converged within the predetermined tolerance of 1 percent error. One of the neural network solution of the strain hardening is shown for one temperature in Figure 5, and compared at the several FGM volume fractions with the teach data. A sufficiently reliable accuracy is seen to be acquired for the subsequent analysis.

Thus educated algorithm was embedded in the finite element code for the fracture analysis of FGM structure. The conventional incremental thermo-elastoplastic constitutive law, which accounts for the temperature dependence of the material properties, is employed for the thermal shock analysis. The thermoelastic material properties for the FGM is determined with the use of the spherical grain model by Kerner[5].

Results

The present finite element procedure with the micromechanics analysis and the neural network algorithm were used in application to the thermal shock analysis of a two dimensional section of an inner-cracked FGM pipe. The material component continuously varies from the inside to the outside, with the titanium alloy $Ti-6Al-4V$ to the Zirconia ZrO_2. The variation of the volume fraction of the constituents from one to another is shown in the part of Figure 6, where x is the distance the inner wall and L the thickness of the pipe. The pipe was initially subjected to the temperature of 1000℃ with the pressure of 50MPa inside. And at time 0, the inner surface is subjected to a thermal shock of 700℃. The transient temperature variation through the thickness was determined by a finite difference method, and is shown in Figure 7 for one case of material grading.

At the stand point that the fracture stability of the highly inhomogeneous material as the present is governed by the material and the deformation state of the crack-tip, the best suited fracture parameter, T* integral[6,7], was employed for the crack assessment. T* is physically an energy flow rate out from the crack-tip. Also, the integral parameter provides the path independence even for the present inhomogeneous material, the temperature, and the history dependent loading regime.



Volume fractions:

$V_2 = (1 - \frac{x}{L})^Q$: $Ti-6Al-4V$

$V_1 = 1 - V_2$: ZrO_2

Figure 6. FGM pipe with internal crack.

During the thermal shock, the variations of the crack-tip severity are calculated in the present analysis and shown in Figure 7 for the various material gradings of the power coefficient q. For q = 0.5 and q = 1.0, the plastic effect of the FGM is recognized noting that the crack-tip severity with T* in the elastoplastic regime is mitigated in comparison with that in the elastic regime. But, it is not always the case, ie. for q = 2.0 the crack is more severe in the elastoplastic case than the elastic case, which means that the elastoplastic effect does not always mitigate the severity of the crack in the FGM.

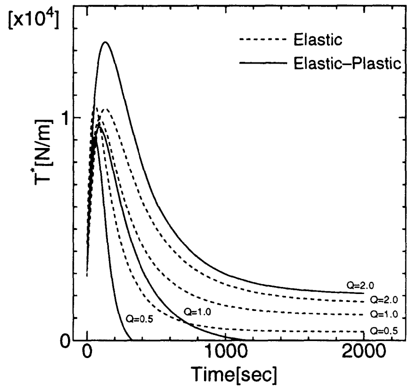


Figure 7. Fracture severity of FGM pipe crack subjected to thermal shock.

Closure

An elastoplastic constitutive law based on the equivalent inclusion method and the mean field theory for the functionally graded material was shown. Also shown is the computational constitutive law by based on the micromechanics analysis and the neural network algorithm. When the case that the volume fraction of the inclusion is large, the theory, which does not account for the stress interaction between inclusion grains incurs inaccuracies quite a little. Whereas, the present model with the neural network has the sufficient reliability for arbitrary temperature and the volume fractions with no ambiguities for the analysis of the present class of problem.

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