Abstract

The objective of the present study is to establish the experimental modeling process of the nonuniform deformation behavior of heterogeneous materials. For this purpose, the constant stress moment, which is the work conjugate quantity of the constant strain gradient for the finite volume evaluation region, is introduced. The proposed stress moment can be evaluated from the stress field. The extended constitutive equation that relates the strain, stress, strain gradient, and stress moment is then formulated to predict the nonuniform deformation behavior of heterogeneous materials. In order to confirm that the proposed method is appropriate to represent the nonuniform deformation, finite element method (FEM) simulations of bending of macroscopically and microscopically heterogeneous materials were performed. The proposed method could predict the bending deformation of macroscopically heterogeneous material as precisely as the homogeneous case because the distribution of the heterogeneity is introduced in the extended constitutive equation. A bending simulation of a laminated cantilever was then performed using the extended constitutive equation for the microscopically heterogeneous material. The proposed method was capable of representing the analytically verified size-dependent bending deformation of the laminated cantilever.

Keywords: Applied mathematics, Mechanical engineering, Materials science
1. Introduction

It is very important to evaluate and model the nonuniform deformation of engineering materials in the study of the continuum mechanics of solids. When the object material is a homogeneous material, the conventional finite element method (FEM) procedure can be applied to predict the nonuniform deformation. However, engineering materials usually have a microscopic heterogeneity that affects nonuniform deformation especially when the size difference between macro- and microstructures is small, e.g., the stress concentration around the corner of a small-sized component, the necking of a thin wire, and the crack tip plastic zone. To accurately predict the mechanical behavior in such a situation, the response to the nonuniform deformation characterized by the material heterogeneity should be determined.

Recently, the nonuniform deformation of various materials has been precisely evaluated using digital image correlation (DIC). The main concept of DIC was proposed by Sutton et al. (1983, 1986), and many related papers have been published (Raabe et al., 2001; Parsons et al., 2004; Uchida and Tada, 2011; Le Cam, 2012). Furthermore, a method for evaluating the strain and stress fields has been established based on the DIC-FEM coupling method (Uchida et al., 2017). The stress field can also be obtained in the process of the virtual field method (Avril et al., 2008; Wang et al., 2016), which is proposed to characterize the material parameters. These studies enable the evaluation of the stress and strain fields under nonuniform deformation, and provide valuable information for the modeling of the nonuniform deformation behavior of engineering materials. The future modeling process of mechanical behavior of the engineering materials may shift to the experimental determination of not only the response to the strain but also the response to nonuniform deformation.

To directly use the stress and strain fields in the modeling of nonuniform deformation, physical quantities characterizing these fields should be included in the constitutive equation of the material. The strain gradient is usually employed as a barometer of nonuniform deformation. In this case, its work conjugate higher-order stress should be introduced in the constitutive equation. Constitutive models, including the strain gradient and its work conjugate higher-order stress, have been developed in nonlocal continuum mechanics. The development of a framework for nonlocal continuum mechanics started in the 19th century. The Cosserat brothers (1909) described a nonlocal elastic deformation behavior containing a rotation gradient by introducing the couple stress. In the 1960s, Toupin (1962), Mindlin (1964) and Mindlin and Eshel (1968) developed more general gradient theories for elastic deformation behavior. After the 1980s, the strain gradient theory was extended to plastic deformation, and various engineering problems were studied using the gradient theory (Aifantis, 1987, 1992; Fleck and Hutchinson, 1993, 1997).
Micro- to macroscopic modeling of nonlocal deformation was also studied using the second-order homogenization method (Kouznetsova et al., 2002, 2004). Although well-defined higher-order stresses were introduced in those studies, it is difficult to validate them by the direct comparison with the experimental result because the experimental evaluation process of the higher-order stress has not yet been established. The higher-order stress should be easily evaluated from experimental result similar to the stress, strain and strain gradient in order to model the nonlocal deformation behavior of arbitrary engineering materials.

The final goal of this study is an establishment of the experimental modeling process of the nonuniform deformation of engineering materials. In this framework, the concept of the resistance to nonuniform deformation is introduced using the 1st and 2nd moment of the material’s stiffness. First, we consider the finite volume evaluation region from the object material. The strain field of the evaluation region is described using the 0th- and 1st-order gradients of strain field, \( \varepsilon^0 \) and \( \gamma^0 \), respectively, which are assumed as constant in the evaluation region. Next, the 0th and 1st moment of stress field, \( \sigma^0 \) and \( \mu^0 \), are employed for the work conjugated quantities of \( \varepsilon^0 \) and \( \gamma^0 \), respectively. Hereafter, \( \varepsilon^0, \gamma^0, \sigma^0 \) and \( \mu^0 \) are referred to as strain, strain gradient, stress and stress moment. The stress moment, which corresponds to the higher-order stress proposed in this study, can be easily evaluated from experimentally obtained stress field.

When the stiffness \( D \) of the evaluation region is known, the extended constitutive equation, which relates the strain, stress, strain gradient, and stress moment, can be constructed using the 1st and 2nd moments of stiffness. For the homogeneous evaluation region, the 1st moment of stiffness becomes zero, and the 2nd moment of stiffness can be written as a product of the stiffness \( D \) and the 2nd moment of volume \( J; D \otimes J \). On the other hand, they are nonzero and not \( D \otimes J \) for the heterogeneous evaluation region. Although the heterogeneity of the material is difficult to characterize experimentally, the 1st and 2nd moments of stiffness can be estimated by comparing the experimentally obtained stress and strain fields of the evaluation region. In this work, we attempt to model the nonuniform deformation characterized by the material heterogeneity based on above concept.

The first important issue of this framework is to prove that the proposed method is appropriate for the description of nonuniform deformation of the heterogeneous material. In this paper, two simple FEM simulations of nonuniform deformation are demonstrated to validate the proposed method. In the usual FEM process, the simulation object is firstly meshed using finite elements and the material parameters are assigned to all the integration points. When the object material has a heterogeneously distributed strength or the material parameter developed by deformation is assigned to the integration point, the simulation result depends on the mesh division. The improvement of a mesh dependency by the proposed method is firstly shown in
the bending simulation of the elastically heterogeneous cantilever. Next, we demonstrate that the proposed method can represent the scale-dependent nonuniform deformation of the material having a heterogeneous microstructure. The formulation process of this demonstration is based on a second-order homogenization without the microscopic fluctuation. This represents the simple modeling method of the scale-dependent mechanical behavior of the microscopically heterogeneous material. The scale-dependent bending properties of a two-phase laminated cantilever are represented using the proposed method.

2. Theory

2.1. Introduction of quantities

This section introduces the physical quantities for describing the nonuniform deformation of a material. First, we define an evaluation region having a finite volume $V$ with center $x_i^0$ as shown in Fig. 1. The coordinates $x_i$ in this volume satisfy Eq. (1) as

$$\int_V (x_i - x_i^0) dV = \int_V \Delta x_i dV = 0.$$  

We assume that the displacement field in this region can be expressed by a second-order Taylor series expansion as Eq. (2).

$$u_i(x) = u_i^0 + u_{ij}^0 \Delta x_j + \frac{1}{2} u_{ijk}^0 \Delta x_j \Delta x_k,$$  

where $u_i^0$, $u_{ij}^0$, and $u_{ijk}^0$ are the 0th-, 1st-, and 2nd-order gradients of the displacement at the center of the evaluation region, respectively, and are constant in the region. Therefore, the field of the displacement gradient can be expressed by Eq. (3).

$$u_{ij}(x) = u_{ij}^0 + u_{ijk}^0 \Delta x_k.$$  

Fig. 1. Schematics of deformation of a finite volume evaluation region in an object.
The strain field is given by Eq. (4).

\[ \varepsilon_{ij}(x) = \varepsilon_{ij}^0 + \gamma_{ijk}^0 \Delta x_k, \]  

(4)

where \( \varepsilon_{ij}^0 \) is the symmetric part of \( u_{ij}^0 \), and \( \gamma_{ijk}^0 = u_{ijk}^0 = u_{i,kj}^0 = \gamma_{ikj}^0 \) respectively.

When the virtual strain field \( \delta \varepsilon_{ij}(x) \) is also described by Eq. (4), the virtual work per unit volume \( \delta w \) for the evaluation region is given by Eq. (5).

\[ \delta w = \frac{1}{V} \int \left( \delta \varepsilon_{ij} + \delta \gamma_{ijk} \Delta x_k \right) \sigma_{ij}(x) dV \]

\[ = \delta \varepsilon_{ij}^0 \frac{1}{V} \int \sigma_{ij}(x) dV + \delta \gamma_{ijk}^0 \frac{1}{V} \int \Delta x_k \sigma_{ij}(x) dV \]

\[ = \delta \varepsilon_{ij}^0 \sigma_{ij}^0 + \delta \gamma_{ijk}^0 \mu_{kij}^0. \]

(5)

The quantities work conjugated with strain and strain gradient are defined by the 0th and 1st moments of the stress, which are referred to as stress and stress moment, as Eqs. (6) and (7);

\[ \sigma_{ij}^0 \equiv \frac{1}{V} \int \sigma_{ij}(x) dV, \]

(6)

\[ \mu_{kij}^0 \equiv \frac{1}{V} \int \Delta x_k \sigma_{ij}(x) dV. \]

(7)

Note that \( \sigma_{ij}^0 \) and \( \mu_{kij}^0 \) are also constants in the evaluation region. Therefore, the stress moment, which is the higher-order stress proposed in this study, can be easily evaluated from experimentally obtained stress field only. When the equation relating the strain \( \varepsilon_{ij}^0 \), strain gradient \( \gamma_{ijk}^0 \), stress \( \sigma_{ij}^0 \) and stress moment \( \mu_{kij}^0 \) is given, we can predict the deformation behavior of the material under the nonuniform deformation based on the virtual work principle using Eq. (5).

Note that the stress \( \sigma_{ij}^0 \) and strain \( \varepsilon_{ij}^0 \) employed in this study depend on the size of the evaluation region under nonuniform deformation. However, introduction of the strain gradient \( \gamma_{ijk}^0 \) and stress moment \( \mu_{kij}^0 \) reduces change in the energy estimation for different size of evaluation regions even under nonuniform deformation. Introduction of higher-order gradients of strain and those work-conjugate stresses gives the more accurate result. On the other hand, stress and strain also vary when the target evaluation region has material heterogeneity, e.g., a multi-phase structure in the composite, a polycrystalline structure in the metal, and a dislocation distributed structure in the crystal. In the present study, we attempt to represent nonuniform deformation measured by the experiment. Therefore, the size of the evaluation
region is assumed to correspond to that used for stress and strain fields measurement in the experiment.

2.2. Extended constitutive equations for macroscopically heterogeneous materials

In this section, the extended constitutive equation that relate the strain, stress, strain gradient, and stress moment defined in Section 2.1 are formulated for the elastic material. When the strain field given by Eq. (4) is applied to a macroscopically heterogeneous material, the actual stress field $\sigma_{ij}(x)$ at an arbitrary point is given by Eq. (8).

$$\sigma_{ij}(x) = D^{e}_{ijkl}(x)\left(\epsilon_{kl}^{0} + \gamma_{klm}^{0}\Delta x_{m}\right),$$

where $D^{e}_{ijkl}(x)$ is the elastic modulus tensor. The virtual work per unit volume, $\delta w$, is given by Eq. (9).

$$\delta W = \left( \delta \epsilon_{ij}^{0} \quad \delta \gamma_{ij}^{0} \right) \left[ D^{(11)}_{ijkl} \quad D^{(12)}_{ijkl} \quad D^{(21)}_{ijkl} \quad D^{(22)}_{ijkl} \right] \left\{ \epsilon_{kl}^{0} \quad \gamma_{klm}^{0} \right\},$$

where $D^{(11)}_{ijkl} = \int D^{e}_{ijkl}(x) dV / V$, $D^{(12)}_{ijkl} = \int D^{e}_{ijkl}(x) \Delta x_{m} dV / V = D_{mijkl}$, and $D^{(21)}_{ijkl} = \int \Delta x_{m} D^{e}_{ijkl}(x) \Delta x_{m} dV / V$. The 1st and 2nd moments of the stiffness, $D^{(12)}_{ijkl}$, $D^{(21)}_{ijkl}$ and $D^{(22)}_{ijkl}$ include information of distribution of the strength in the evaluation region. Therefore, Eq. (9) can accurately evaluate the virtual work for nonuniform deformation of the evaluation region of the heterogeneous material.

When the elastic property is uniform in the evaluation region, Eq. (9) can be simplified. In this case, the 1st moment of the stiffness are zero, and the stress $\sigma_{ij}^{0}$ and stress moment $\mu_{mnij}^{0}$ are given by Eqs. (10) and (11).

$$\sigma_{ij}^{0} = \frac{1}{V} \int \sigma_{ij}(x) dV = D^{e}_{ijkl} \epsilon_{kl}^{0},$$

$$\mu_{mnij}^{0} = \frac{1}{V} \int \Delta x_{m} \sigma_{ij}(x) dV = D^{e}_{ijkl} J_{mn}^{0} \gamma_{klm}^{0}.$$
2.3. Extended constitutive equations for microscopically heterogeneous materials

Even though mechanical properties are macroscopically uniform, engineering materials generally have the microscopic heterogeneity, and it affects the deformation behavior of the materials. In this section, the extended constitutive equation for microscopically heterogeneous materials is proposed by introducing a periodic microstructure with the finite volume. The proposed constitutive equation can evaluate the size effect of the material. The formulation process in this section is similar to the second-order homogenization (Kouznetsova et al., 2002 and 2004) without the microscopic fluctuation.

We consider the microscopically heterogeneous material as shown in Fig. 2. The microscopically heterogeneous material is modeled using the periodic structure with a finite volume $Y$, microscopically periodic coordinate for the unit cell, $\Delta x_i^m$, and the distance between centers of $I$ th unit cell and the macroscopic evaluation region, $\Delta x_i^{M(I)}$ (see Fig. 2). In a similar manner to section 2.1, we consider the strain and stress fields on the macroscopic evaluation region with finite volume $V$. The relationship between macro- and microscopic coordinates is given by Eq. (13).

$$x_i = x_i^0 + \Delta x_i^{M(I)} + \Delta x_i^m = x_i^m + \Delta x_i^{M(I)},$$  \hspace{1cm} (13)

where $x_i^m$ is microscopic coordinate for the unit cell located at the center of the evaluation region. The quantity defined on this coordinate are independent of the location of unit cell, namely, the quantity is periodic in the evaluation region. The constitutive equation on the material point $x$ is given by Eq. (14).

$$\sigma_{ij}(x) = D_{ijkl}(x^m)\varepsilon_{kl}(x),$$  \hspace{1cm} (14)

where $D_{ijkl}(x^m)$ is the periodic elastic modulus field in the unit cell. The proposed stress and stress moment given by Eqs. (6) and (7) are then obtained as Eqs. (15) and (16).

Fig. 2. Microscopically heterogeneous material.
\[
\sigma_{ij}^0 = \frac{1}{V} \int V D_{ijkl}(x^n) \left( \epsilon_{ki}^0 + \gamma_{kln}^0 \Delta x_m \right) dV, \quad (15)
\]

\[
\mu_{ij}^0 = \frac{1}{V} \int V \Delta x_n D_{ijkl}(x^n) \left( \epsilon_{ki}^0 + \gamma_{kln}^0 \Delta x_m \right) dV. \quad (16)
\]

Because \( D_{ijkl}(x^n) \) is periodic, these equations can be simplified. First, the number of the microscopic structures contained in a macroscopic evaluation region is obtained as

\[
N = \frac{V}{V'} \quad (17)
\]

Then, the 1st moment of the macroscopic evaluation region is evaluated using the 1st moment of the unit cell as

\[
\frac{1}{V} \int V \Delta x_i dV = \frac{1}{V} \int V \left( \Delta x_i^{M(I)} + \Delta x_i^n \right) dV = \frac{1}{V} \left( Y \sum_{l=1}^{N} \Delta x_i^{M(l)} + N \int \Delta x_i^m dY \right) = 0. \quad (18)
\]

Since the 1st moment of the unit cell \( \int \Delta x_i^m dY \) is zero, we obtain

\[
\sum_{l=1}^{N} \Delta x_i^{M(l)} = 0. \quad (19)
\]

Next, we consider the 2nd moment of the macroscopic average volume;

\[
\frac{1}{V} \int V \Delta x_i \Delta x_j dV = \frac{1}{V} \int V \left( \Delta x_i^{M(I)} + \Delta x_i^n \right) \left( \Delta x_j^{M(I)} + \Delta x_j^n \right) dV. \quad (20)
\]

Substituting Eqs. (17), (18), and (19) into Eq. (20), we obtain Eq. (21).

\[
\frac{1}{N} \sum_{l=1}^{N} \Delta x_i^{M(l)} \Delta x_j^{M(l)} = J_{ij} - Y^Y_{ij}, \quad (21)
\]

where \( J_{ij}^Y = \int V \Delta x_i^m \Delta x_j^m dY / Y \) are the 2nd moment of the average volume of the unit cell. The average, the 1st and 2nd moments of \( D_{ijkl}(x^n) \) are simplified using above equations as Eqs. (22), (23), and (24).

\[
\frac{1}{V} \int V D_{ijkl}(x^n) dV = \frac{1}{V} \sum_{l=1}^{N} \int Y D_{ijkl}(x^n) dY = \frac{1}{V} \int Y D_{ijkl}(x^n) dY = D_{ijkl}^{(11)}, \quad (22)
\]
\[
\frac{1}{V} \int D_{ijkl}(x^n) \Delta x_m dV = \frac{1}{Y} \int D_{ijkl}(x^n) \Delta x_m dY = D^{(12)}_{ijklmn} = D^{(21)}_{ijklmn},
\]

(23)

\[
\frac{1}{V} \int \Delta x_p D_{ijkl}(x^n) \Delta x_m dV = \tilde{D}^{(11)}_{ijkl} (J_{nm} - J^Y_{nm}) + \frac{1}{Y} \int \Delta x_m D_{ijkl}(y) \Delta x_p dY
\]

\[= \tilde{D}^{(11)}_{ijkl} (J_{nm} - J^Y_{nm}) + D^{(22)}_{ijklmn}.\]

(24)

Finally, the extended constitutive equation is given by Eq. (25).

\[
\begin{bmatrix}
\sigma^0_{ij}
\end{bmatrix}
= \begin{bmatrix}
\tilde{D}^{(11)}_{ijkl}
\tilde{D}^{(12)}_{ijklmn}
\end{bmatrix}
\begin{bmatrix}
\varepsilon^0_{ij}
\end{bmatrix}
+ \begin{bmatrix}
\varepsilon^0_{ij}
\gamma^0_{ij}
\end{bmatrix},
\]

(25)

This equation contains the dimension of microscopic length scale in \(D^{(12)}_{ijklmn}, \tilde{D}^{(21)}_{ijklmn}, J^Y_{nm}\), and \(D^{(22)}_{ijklmn}\).

2.4. Two-dimensional description of discretized extended constitutive equation

Two-dimensional discretization of the extended constitutive equation proposed in section 2.1 is shown here to perform the FEM simulation. The strain and strain gradient for a finite volume used in Eq. (4) is described by vector form as Eqs. (26) and (27).

\[
\begin{bmatrix}
\varepsilon^0
\end{bmatrix}
= \begin{bmatrix}
\varepsilon^0_{11}
\varepsilon^0_{22}
2\varepsilon^0_{12}
\end{bmatrix}^T,
\]

(26)

\[
\begin{bmatrix}
\gamma^0
\end{bmatrix}
= \begin{bmatrix}
\gamma^0_{111}
\gamma^0_{222}
\gamma^0_{122}
\gamma^0_{211}
\gamma^0_{112}
\gamma^0_{221}
\end{bmatrix}^T.
\]

(27)

Similarly, the stress in Eq. (6) and stress moment in Eq. (7) are also described in vector form as Eqs. (28) and (29).

\[
\begin{bmatrix}
\sigma^0
\end{bmatrix}
= \begin{bmatrix}
\sigma^0_{11}
\sigma^0_{22}
\sigma^0_{12}
\end{bmatrix}^T,
\]

(28)

\[
\begin{bmatrix}
\mu^0
\end{bmatrix}
= \begin{bmatrix}
\mu^0_{111}
\mu^0_{222}
\mu^0_{122}
\mu^0_{211}
\mu^0_{112}
\mu^0_{221}
\end{bmatrix}^T.
\]

(29)

The 1st and 2nd moments of stiffness in Eq. (9) are then described in matrix form as Eqs. (30), (31), (32), and (33).

\[
\begin{bmatrix}
D^\varepsilon^{(11)}
\end{bmatrix}
= \begin{bmatrix}
D^\varepsilon_{1111}^{(11)}
D^\varepsilon_{1122}^{(11)}
D^\varepsilon_{2211}^{(11)}
D^\varepsilon_{2222}^{(11)}
D^\varepsilon_{1211}^{(11)}
D^\varepsilon_{1222}^{(11)}
D^\varepsilon_{1212}^{(11)}
D^\varepsilon_{1221}^{(11)}
D^\varepsilon_{1212}^{(11)}
D^\varepsilon_{2212}^{(11)}
\end{bmatrix},
\]

(30)
The extended constitutive equation is then discretely described as Eq. (34)

\[
\begin{pmatrix}
\sigma^0 \\
\mu^0
\end{pmatrix} = \begin{bmatrix}
D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} + D^{(12)} \\
D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} + D^{(12)} \\
D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} + D^{(12)} \\
D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} + D^{(12)} \\
D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} & D^{(12)} + D^{(12)}
\end{bmatrix}
\begin{bmatrix}
\mathbf{e}^0 \\
\mathbf{e}^0
\end{bmatrix}.
\]  

(34)

In the computation, the evaluation region in Fig. 1 corresponds to a finite element. Therefore, the strain and strain gradient for the evaluation region is calculated using the displacement vectors on the nodal points of the finite element. Now, the direct transformation equations from the displacements on the nodal points to the strain and strain gradient for the element are explained here. In conventional FEM, the displacement field \(u_i(x)\) in the finite element is approximated by the summation of the product of shape function \(S^{(f)}(x)\) and displacement vector \(u^{(f)}_i\) for \(I\) th nodal point as Eq. (35).

\[
u_i(x) = \sum_{i=1}^{N} S^{(f)}(x) u^{(f)}_i,
\]

(35)

where \(N\) is the number of the nodal point for an element. Therefore, the strain and strain gradient for the center of the element is calculated by Eqs. (36) and (37).
\[ \gamma_{ij}^{0} = \gamma_{ij}(x_0) = \sum_{I=1}^{N} \frac{\partial^2 S_{ij}^{(I)}}{\partial x_i \partial x_j} (x_0) u_i^{(I)} = \sum_{I=1}^{N} \frac{\partial^2 S_{ij}^{(I)}}{\partial x_i \partial x_j} u_i^{(I)}. \]  

(37)

Since the shape function is usually represented using the natural coordinate system, the strain is calculated as Eq. (38).

\[ \varepsilon_{ij}^{0} = \varepsilon_{ij}(x_0) = \sum_{I=1}^{N} \frac{\partial S_{ij}^{(I)}}{\partial x_j} (x_0) u_i^{(I)} = \sum_{I=1}^{N} \frac{\partial S_{ij}^{(I)}}{\partial x_j} u_i^{(I)}, \]  

(36)

\[ \varepsilon_{ij}^{0} = \sum_{I} \omega_{ij} \frac{\partial S_{ij}^{(I)}}{\partial x_j} u_i^{(I)} = \sum_{I} B_{ij}^{(I)} u_i^{(I)}, \]  

(38)

or in matrix form as Eq. (39)

\[ \{\varepsilon^{0}\} = \sum_{I} \begin{bmatrix} B_{1}^{(I)} & 0 \\ 0 & B_{2}^{(I)} \\ B_{2}^{(I)} & B_{1}^{(I)} \end{bmatrix} \{u^{(I)}\} = \sum_{I} [B^{(I)}] \{u^{(I)}\}, \]  

(39)

where \( \omega_{ij} \) is an inverse of the Jacobian matrix given by Eq. (40),

\[ \phi_{ij} = \frac{\partial x_i}{\partial \xi_j} = \sum_{I} \frac{\partial S_{ij}^{(I)}}{\partial \xi_j} x_j^{(I)}, \]  

(40)

and \( x_j^{(I)} \) is the coordinate of the \( I \)th nodal point. The 2nd-order gradient of the displacement field using the natural coordinate system is then calculated as Eq. (41).

\[ \frac{\partial^2 u_j^{0}}{\partial \xi_j \partial \xi_m} = \phi_{ij} \phi_{jm} \gamma_{ij}^{0} + \omega_{ij} \frac{\partial x_m}{\partial \xi_j} \frac{\partial u_j^{0}}{\partial \xi_m}. \]  

(41)

Therefore, the strain gradient for the finite element is calculated as Eq. (42).

\[ \gamma_{ij}^{0} = \omega_{ij} \omega_{jm} \left( \frac{\partial^2 u_j^{0}}{\partial \xi_j \partial \xi_m} - \omega_{ij} \frac{\partial^2 x_m}{\partial \xi_j \partial \xi_m} \right) \]  

\[ = \sum_{I} \omega_{ij} \omega_{jm} \left( \frac{\partial^2 S_{ij}^{(I)}}{\partial \xi_j \partial \xi_m} - \omega_{ij} \sum_{I} \frac{\partial^2 S_{ij}^{(I)}}{\partial \xi_j \partial \xi_m} x_j^{(I)} \right) u_i^{(I)} \]  

(42)

or in matrix form as Eq. (43).
\[ \{\gamma_0\} = \sum_{I} \begin{bmatrix} C^{(I)}_{11} & 0 \\ 0 & C^{(I)}_{22} \\ C^{(I)}_{22} & 0 \\ 0 & C^{(I)}_{11} \\ C^{(I)}_{12} & 0 \\ 0 & C^{(I)}_{21} \end{bmatrix} \{u^{(I)}_1\} = \sum_{I} \begin{bmatrix} C^{(I)} \end{bmatrix} \{u^{(I)}\}. \] (43)

The matrices \([B^{(I)}]\) and \([C^{(I)}]\) are the transformation matrices from the displacement of nodal points to the strain and strain gradient of the element, respectively. Finally, the virtual work of Eq. (5) for the finite region can be described using the nodal displacement as Eq. (44).

\[ \delta w = \sum_{I} \{\delta u^{(I)}\} \left( [B^{(I)}]^T [C^{(I)}]^T \right) \left[ \begin{bmatrix} D^{(11)} \\ D^{(21)} \\ D^{(12)} \\ D^{(22)} \end{bmatrix} \right] \left\{ \begin{bmatrix} [B^{(I)}] \\ [C^{(I)}] \end{bmatrix} \right\} \{u^{(I)}\}. \] (44)

The vector, which is a work conjugate quantity of the virtual displacement \(\{\delta u^{(I)}\}\), is defined as a nodal force of the finite region as Eq. (45).

\[ \{f^{(I)}\} = \left( [B^{(I)}]^T [C^{(I)}]^T \right) \left[ \begin{bmatrix} D^{(11)} \\ D^{(21)} \\ D^{(12)} \\ D^{(22)} \end{bmatrix} \right] \left\{ \begin{bmatrix} [B^{(I)}] \\ [C^{(I)}] \end{bmatrix} \right\} \{u^{(I)}\} 
= [B^{(I)}]^T \{\sigma^0\} + [C^{(I)}]^T \{\mu^0\}. \] (45)

As shown in Eq. (45), the nodal force in the proposed method is generated by the stress and stress moment of the finite region. The displacement field satisfying the equilibrium between inner and outer forces of all nodal points is solved under the boundary condition.

### 3. Results and discussion

#### 3.1. Bending of macroscopically heterogeneous materials

To validate the proposed method, two simple FEM examples, in which we can obtain the analytical solution, are demonstrated in sections 3.1 and 3.2. In the case of the homogeneous material, the accuracy of the proposed method should coincide with that of the conventional FEM calculation with the second-order element because the second-order element can evaluate the strain gradient in the finite element. Therefore, we can validate the proposed method when same results are obtained in the simulation of nonuniform deformation of the homogeneous material. On the other hand, the proposed method can predict the nonuniform deformation behavior of the heterogeneous material more accurately than the conventional FEM since the distribution of the stiffness in the evaluation region is included in the extended constitutive equation. In section 3.1, simulations of the bending of homogeneous and heterogeneous cantilevers shown in Fig. 3 were demonstrated.
The distributions of the Young’s modulus in thickness direction were introduced by different functions given by Eqs. (46), (47), and (48), and they are shown in Fig. 3 (b).

Material 0: 
\[ E(x_2) = E_0, \]  
(46)

Material 1: 
\[ E(x_2) = E_0 + E_1 x_2 / h, \]  
(47)

Material 2: 
\[ E(x_2) = E_0 + \frac{1}{2} E_2 \left( \frac{x_2}{h} \right)^2. \]  
(48)

The Young’s modulus in material 0 was uniform whereas that in materials 1 and 2 were distributed by a linear and a quadratic functions along the thickness direction, respectively. A uniformly distributed load \( w l / b = -10 \) N was applied to the cantilever with \( l \) in length, \( h \) in thickness, and \( b \) in width. According to the Timoshenko beam theory (Timoshenko, 1930), the deflection on the free end of the cantilever, on which the uniformly distributed load is applied, can be analytically obtained by Eq. (49).

\[ v_A = \frac{w l^4}{8EI} + \frac{wl^2}{2GA}. \]  
(49)

where \( EI = \int_A E(x_2)x_2^2 dA / A \) is the average bending stiffness, \( G \) is an average of the shear modulus, \( A \) is the area of the beam, and \( \alpha \) is the shear modification factor \((\alpha = 1.5 \) for the rectangular cross section). The average bending stiffness for materials 0, 1, and 2 is as Eqs. (50), (51), and (52).

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**Fig. 3.** Model of the macroscopically heterogeneous cantilever. (a) boundary condition for the cantilever, and (b) distribution of the Young’s modulus.
Material 0: 
\[ EI = \frac{E_0 bh^3}{12}, \]  
(50)

Material 1: 
\[ EI = \frac{E_0 bh^3}{12} \left(1 - \frac{E_1^2}{12E_0^2}\right), \]  
(51)

Material 2: 
\[ EI = \frac{E_0 bh^3}{12} \left(1 + \frac{3E_2}{40E_0}\right). \]  
(52)

To investigate the dependency of the simulation accuracy on the mesh division, four different mesh divisions, namely, \(1 \times 10 \times 2, 2 \times 20 \times 2, 5 \times 50 \times 2, \) and \(10 \times 100 \times 2\), as shown in Fig. 4, were given to the cantilever. Since a strain gradient has to be evaluated to construct the extended constitutive equation, a 6-node triangle element was employed for the finite element. In order to evaluate the validity and accuracy of the proposed method, conventional FEM simulations using the same conditions were also performed, and the results obtained from both methods and the analysis result given by Eq. (49) were compared. The two-dimensional simulations were done under the plane stress condition, and the material parameters used were \(E_0 = 100\) GPa, \(\nu = 0.3, E_1/E_0 = 0.5, E_2/E_0 = -0.5, l = 10\) mm and \(h = 1\) mm.

The relationships between the normalized deflection of the free end, \(v_A/h\), and the normalized representative mesh size, \(d/h\) (see Fig. 4), for different mesh divisions are shown in Fig. 5. The analysis result for each material is also shown in the figure. The deflections obtained from both the proposed and conventional simulations come near to the analysis result for the finer mesh division in all materials. Results of the proposed method and the conventional FEM coincides for material 0. This result indicates that introduced stress moment and extended constitutive equation correctly estimate the energy required to generate the nonuniform deformation of the homogeneous material. Regarding materials 1 and 2, there are large differences between
the simulation and analysis results for the conventional FEM models with coarser meshes. This tendency is stronger in material 2, which has a more complex heterogeneity than material 1. On the other hand, the proposed method can predict the deflection of the macroscopically heterogeneous cantilevers more accurately than the conventional FEM. To show the difference more clearly, the relationships between ratios of the simulation and analysis results and the normalized mesh size are plotted in Fig. 6. As shown in the figure, the mesh dependence of the simulation
is enlarged with the increase in the complexity of the heterogeneity in the conventional FEM, whereas with the proposed method the results agree for all materials. Therefore, the effect of macroscopic heterogeneity of materials can be removed from the computational simulation by introducing the extended constitutive equation proposed in the present study.

3.2. Bending of microscopically heterogeneous materials

In section 3.2, the nonuniform deformation behavior of a microscopically heterogeneous material is investigated. The laminated cantilever, in which two different materials are laminated in the thickness direction as shown in Fig. 7, is considered as the microscopically heterogeneous material. The laminated cantilever is modeled as a periodic structure of the unit structure shown in Fig. 7 (b). The local bending stiffness of the two-phase unit structure with respect to the neutral axis of the structure, $EI_Y$, is given by Eq. (53).

$$EI_Y = \frac{bh_U^3}{12} \left( E_1 + f_0^3 \Delta E \right),$$

where $h_U = h/N$ is the thickness of the unit structure, $N$ is the number of the unit structure in the thickness direction, $E_0$ and $E_1$ are the Young’s moduli of materials 0 and 1, $f_0$ is the volume fraction of material 0, and $\Delta E = E_0 - E_1$. The bending stiffness of the whole structure, $EI_X$, can be calculated by Eq. (54).

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Fig. 7. Model of the microscopically heterogeneous cantilever. (a) boundary condition for the laminated cantilever and (b) unit structure.
\[ EI_X = \sum_{I=1}^{N} \left( EI_y + E_A^{(I)} A^{(I)} \right), \]

where \( E \) is the average Young’s modulus, \( \lambda_{sg}^{(I)} \) is the distance between the neutral axes of \( I \)th unit and the whole structure, and \( A^{(I)} \) is the local area of \( I \)th unit structure.

The computational simulation of bending of the laminated cantilever was performed using the extended constitutive equation for the microscopically heterogeneous material shown in Eq. (25). The uniformly distributed load \( wL/b = -10 \)N was given to the laminated cantilevers with different numbers of layers. Different mesh divisions were prepared for each layer-thickness cantilever. In this case, since the unit structure should be smaller than the macroscopic finite element, mesh divisions with \( d \geq h_U \) were used for each lamination cantilever. In a similar manner to section 3.1, two-dimensional simulations were done under the plane stress condition, and the material parameters used in the simulation were \( E_0 = 100 \)GPa, \( \nu = 0.3 \), \( E_1/E_0 = 3 \), \( f_0 = 0.5 \), and \( l/h = 10 \).

The normalized deflections of the free end, \( v_A/h \), for cantilevers with different layer-thickness are shown in Fig. 8. The solid line is the analysis result given by Eq. (49)
with the bending stiffness of Eq. (54), whereas the plots are those obtained by FEM simulations of the proposed method with different mesh divisions. For comparison, the deflection for the case of $N = \infty$, i.e., the homogeneous cantilever with averaged Young’s modulus, is added in the figure by dot line. As depicted in the figure, the deflection predicted by both the simulation and analysis change depending on the layer-thickness of the laminated cantilever. This result shows that the proposed model can qualitatively predict the size effect of nonuniform deformation of a microscopically heterogeneous material. Since the deflection approaches that of the homogeneous cantilever with reduced layer-thickness, the result of the smallest layer-thickness model of each mesh division corresponds to the result of the homogeneous cantilever shown in section 3.1. Therefore, the result of the smallest layer-thickness model with coarser mesh division shows a larger difference than that of the homogeneous material. On the other hand, the difference between the simulation and analysis results for a larger layer-thickness model becomes small even in the coarse mesh model. This result indicates that the use of the extended constitutive equation for the simulation of nonuniform deformation of microscopically heterogeneous materials enables an improved accuracy when the scales of the macroscopic and microscopic evaluation regions are close.

As shown in the sections 3.1 and 3.2, FEM simulation based on the proposed method can accurately predict the bending of both macroscopically and microscopically heterogeneous materials. The effect of such a heterogeneity was rather small in the bending of the elastic material. However, the proposed method may provide useful information in more complex problems e.g., the prediction of the local yielding of an inelastic material, and the evaluation of the fields of stress and strain around the notch. Furthermore, as mentioned in the Introduction, the measurement of the stress moment, which can be evaluated from the stress field, enables the experimental estimation of the effect of heterogeneity of the material. In the next step, the experimental fitting process of nonuniform deformation will be discussed. Strain, stress, strain gradient, and stress moment for the evaluation region can be estimated from fields of stress and strain measured using a full-field measurement methods. Material constants characterizing the material heterogeneity, such as slope and curvature of the stiffness will be employed to relate those quantities.

4. Conclusion

To describe the nonuniform deformation behavior of heterogeneous materials, the extended constitutive equation that relates the stress, strain, strain gradient and stress moment is defined for the finite volume evaluation region. The stress moment proposed in this paper can be evaluated from the stress field. The extended constitutive equation for microscopically heterogeneous materials is also formulated by introducing a periodic microstructure with the finite volume.
The FEM simulation of bending of macroscopically heterogeneous elastic cantilevers was performed using the proposed method. A uniformly distributed load was applied to the homogeneous and heterogeneous elastic cantilevers, and the dependence of the accuracy of the simulation on the mesh division was investigated. The proposed method is able to describe the nonuniform deformation behavior with the same accuracy as the conventional higher-order FEM calculations in the case of a homogeneous elastic material. Although the accuracy of the conventional FEM decreases when the material has macroscopic heterogeneity, the proposed method can predict the bending deformation as accurately as with the homogeneous material.

A bending simulation of the laminated cantilever was then performed using the extended constitutive equation for the microscopically heterogeneous material. The uniformly distributed load was applied to laminated cantilevers with different number of layers. Different mesh divisions were prepared for each layer-thickness cantilever. The deflections predicted by the simulation and analysis vary depending on the layer-thickness of the laminated cantilever. This result shows that the proposed model can qualitatively predict the size effect of nonuniform deformation of a microscopically heterogeneous material.

**Declarations**

**Author contribution statement**

Makoto Uchida: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Yoshihisa Kaneko: Analyzed and interpreted the data; Wrote the paper.

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The authors declare no conflict of interest.

**Additional information**

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