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Coupled, macro–micro modeling for hot deformation and sintering

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Abstract

Coupled, macro–micro modeling is proposed to describe hot deformation and sintering behavior of materials at the elevated temperature. Micro-model for description of microstructure evolution is coupled in the hierarchical structure with the macro-model for deformation of structural members or specimens. Owing to the homogenization theory and the selected unit-cell model, hot pressing as well as hipping processes can be quantitatively described by the present method. Direct coupling among the elasto-creep deformation, the thermal transient and the diffusion process enables us to construct the theoretical frame for quantitative description of various material behavior at the elevated temperature. Numerical examples are shown to demonstrate the validity and effectiveness of the present methodology.

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1. Introduction

Metallic alloys and monolithic ceramics have been developed to have homogeneous microstructure and to improve their intrinsic strength and ductility. In nature, however, most of the plants and the sea-shells are composed of porous-structured or cellular materials [7]. Bamboo has a graded structure in density, resulting in its flexibility in bending. Since fine porous structure leads to high thermal insurance, porous polymers or rubbers have been designed to increase the porosity as much as possible. Hence, most of matters and materials daily used are thought to have their own

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heterogeneous structure as demanded from functional requirement. Their mechanical response can never be precisely described without a rational model of their microstructure. In other words, their mechanical response cannot be described until their microstructure is adequately modeled. Through research and development of optimization theories for geometric design, the homogenization method has become the most reliable tool for this purpose [5].

During materials processing and manufacturing, the starting materials are shaped or often near-net shaped to a designed geometric configuration. To be noticed, their microstructure is also modified or improved to satisfy the design demand. Typical examples can be seen in hot deformation and sintering of materials. Large nonlinear deformation is positively used for shaping of materials at the elevated temperature. During this hot working, original microstructure can be improved to be free from defects through densification, diffusion and joining. During sintering, the discrete connection of particles in the powder compact can be changed to dense continuum. In order to describe quantitatively the above geometric change in shaping as well as the microstructure evolution, macro–micro modeling is also indispensable [14,13,1,3].

Macro–micro modeling is based on the homogenization theory and the finite element method. In the conventional approaches, no coupling was considered between macro- and micro-models. Although nonlinear finite element analysis is effective to describe large deformation of materials in hot working, little data can be provided for microstructure evolution [6]. In addition, very complex constitutive equations are necessary to deal with varying state of materials [9]. While, the Monte-Carlo (MC) methods [11] have been actively used to simulate the mass transportation and grain growth during the holding time in sintering. Although various microstructure evolution can be qualitatively simulated without use of the constitutive equations, no process conditions such as loading and temperature setup can be taken into account.

In the present methodology, a macro-model for deformation and stress analysis of specimens and structural members is coupled in the hierarchical manner with a micro-model for physical description of microstructure evolution [12]. In particular, degradation of materials takes place by generation of voids and defects at the elevated temperature. Mass transportation is activated by diffusion and grain growth. Hence, the above macro–micro modeling must be used to consider the physical coupling behavior even in each level of models, that is, elasto-creep or elasto-plastic model for description of mechanical response, thermal conduction model for description of temperature transients, and diffusion model for description of material evolution. Each model has mutual interaction in the hierarchical structure of the macro–micro modeling. As illustrated in Fig. 1, elasto-creep model is strongly coupled with thermal conduction model, while diffusion model is weakly coupled with the elasto-creep model for multi-scaled modeling in hot deformation and sintering. In the present paper, the above coupled, macro–micro modeling for hot deformation and sintering of materials is theoretically explained with some comments on the basic formulation and the coupling terms. Numerical examples are used to demonstrate the validity and effectiveness of the present methodology. Further advancement in the related research is also discussed.

2. Coupled, macro–micro modeling

Sintering is a process to recover the continuity of matters from the discrete powder compact through the mass diffusion or transportation mechanism. As shown in Fig. 2, since sintering and hot

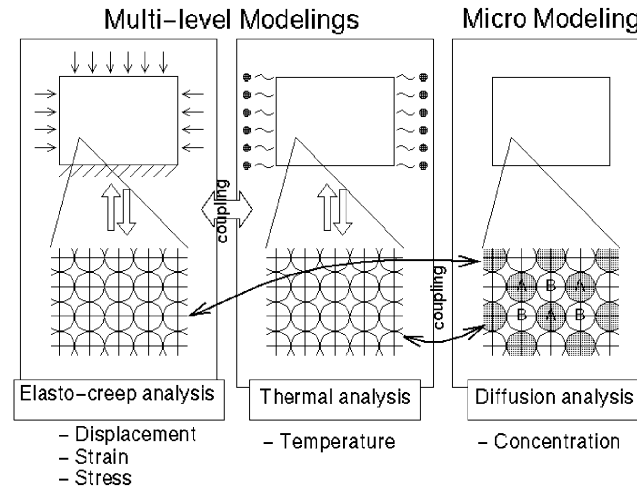


Fig. 1. Coupled, hierarchical modeling for hot deformation and sintering analysis.

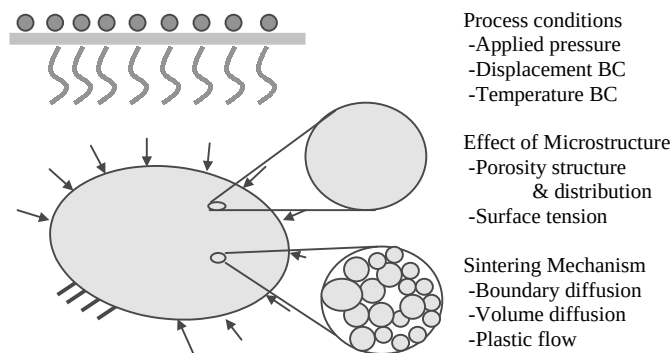


Fig. 2. Heterogeneous advancement of microstructure evolution with densification.

deformation advance heterogeneously with time, local microstructure of materials grows with great difference. This difference reflects on the macroscopic deformation and stress distributions; hence, hierarchical modeling must be constructed with consideration of processing conditions.

The first item required for the coupled macro–micro modeling, to analyze the sintering behavior, is a measure to describe quantitatively the recovery of continuity from powder compact to full dense continuum. Variation of the homogenized stiffness D_{ijkl}^H with time and its distribution in the macro-model is effective to build up this kind of metrics [3]. Since the powder metallurgy (P/M) is a near-net shaping process, the geometric variation of products during P/M process must be accurately analyzed for the final designed shape. Hence, macroscopic change in geometry due to shrinkage must be traced with time. Diffusion process drives nonlinear mass transportation and related mechanical behavior at the elevated temperature. Then, microstructure evolution in sintering is indispensable for a micro-model.

A prototype system is constructed for the coupled, macro–micro modeling in the present paper. To be discussed later, the macro-FEM (finite element method) models for deformation and thermal transients are formulated by using the averaged variational equation or weak form. In the similar manner, the micro-FEM models for deformation, thermal transients and diffusion process, are formulated by using the physical variational equation or weak form. Simultaneous solution of these variational equations for each physical system provides total response of models. Time integration of coupled variational equation systems provides physically coupling effects among deformation, thermal transient and diffusion process.

3. Theory of coupled, macro–micro modeling

Homogenization theory on the basis of the unit cell modeling is used to formulate the above coupled, macro–micro modeling in the frame of the finite element method.

3.1. General frame on the basis of the homogenization theory

Essential contributions in the homogenization theory are briefly summarized in the following. In this theory, the local constitutive structure is thought to have a locally specified periodic unit cell as shown in Fig. 3(a). Hence, every physical variable field on this material support can be expressed by the combination of the averaged part with the local disturbance as depicted in Fig. 3(b). Assuming that the periodicity, ε , should be sufficiently small, every physical field $u(x, y)$ in total can be represented by the following asymptotic expansion in ε :

$$u(x, y) = u^0(x) + \varepsilon u^1(x, y) + \frac{1}{2} \varepsilon^2 u^2(x, y) + \cdots \quad \text{for } y \equiv x/\varepsilon \quad (1)$$

or

$$u(x, y) \approx u^0(x) + \varepsilon u^1(x, y), \quad (2)$$

where $\{u^0, u^1\}$ are functions for the averaged part and disturbance in the coordinates $\{x, y\}$, respectively.

Owing to the periodicity of function u in the y -coordinates, the following two equations are power tool for formulation:

$$\frac{\partial}{\partial x_i} u(x, y) = \frac{\partial u}{\partial x_i} + \frac{1}{\varepsilon} \frac{\partial u}{\partial y_i}, \quad (3)$$

$$\lim_{\varepsilon \rightarrow 0} \int_V u(x, y) dV = \int_V \frac{1}{|Y|} \left(\int_Y u(x, y) dY \right) dV, \quad (4)$$

where Y denotes for a volume of unit cell. Substituting Eq. (1) or (2) to any convex-type variational equation or weak form, $A(u, v) = F(v)$ for $v \in H(V)$, and rearranging it in each term of ε , the following

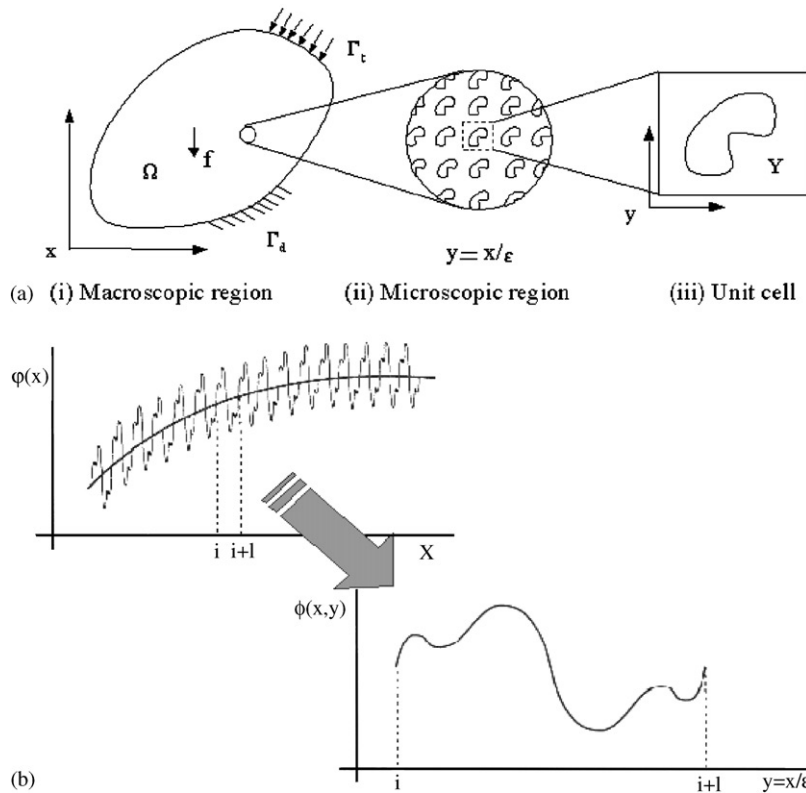


Fig. 3. (a) A frame of multi-scaling in materials using the homogenization theory. (b) Local deviation in the field variable to be embedded into the rationally smoothed distribution.

system of variational equations can be obtained, respectively, for macro- and micro-models:

$$A'(u^0, v) = F'(v) \quad \text{for } v \in H(V) \quad (5)$$

and

$$A''(u^1, v) = F''(v) \quad \text{for } v \in H(Y). \quad (6)$$

In the above, A' and A'' are deduced from $A(u, v)$, and F' and F'' from $F(v)$ through mathematical manipulation, respectively.

In the coupled macro–micro modeling, various field variables and their related governing equations must be formulated into the weak form and solved simultaneously. Table 1 lists typical variables and their governing equations in the coupled analysis for the elasto-creep deformation, the thermal transients and the diffusion process. From the equivalent weak form to the governing equations and the natural boundary conditions in Table 1, the homogenized variational equation (5) for a macro-model and the physical variational equation (6) for a micro-model can be deduced in nearly the same manner. In the following, the finite element formulation for elasto-creep deformation is used as a common frame for variational formulation by the homogenization theory.

Table 1

A list of field variables and related governing equations

	Deformation	Thermal conduction	Diffusion process
Field variable	Displacement (u_i) Strain (ε_{ij}) Stress (σ_{ij})	Temperature (T)	Mass concentration (C)
Governing equations	$\sigma_{ij,j} = 0$ $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ $\varepsilon_{ij}^e = \varepsilon_{ij} - \varepsilon_{ij}^c$ $\varepsilon_{ij}^c = \frac{3}{2} \frac{\bar{\varepsilon}^c}{\bar{\sigma}} S_{ij}$ in V	$\rho C_p \frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x_i^2}$ in V	$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x_i^2}$ in V
Boundary conditions	$u_i = \bar{u}_i$ on S_u $T_i \equiv \sigma_{ij} n_j = \bar{T}_i$ on S_T	$T = \bar{T}$ on S_T $-\kappa \frac{\partial T}{\partial x_n} = \bar{q}$ on S_q	$C = \bar{C}$ on S_C $-D \frac{\partial C}{\partial x_n} = \bar{q}$ on S_q
Initial conditions	$\sigma_{ij} = \varepsilon_{ij} = u_i = 0$ at $t = 0$	$T = T_0(x, y)$ at $t = 0$	$T = C_0(x, y)$ at $t = 0$

Notes: (1) Superscripts “e” and “c” denote the elastic and creep contributions, respectively. (2) S is the surface of V , which is divided into two parts $S_u \cup S_q$, $S_T \cup S_q$ or $S_c \cup S_q$.

3.2. Elasto-creep modeling as a common frame of formulation

Visco-elastic deformation or time-dependent material nonlinearity must be taken into account in order to describe the hot deformation and sintering. Time marching scheme is used to convert the rate form in the governing equation into the incremental formulation. Then, three governing equations for the elasto-creep model in Table 1, are represented by the following:

$$\left. \begin{aligned} \Delta \sigma_{ij,j}^e &= 0, \\ \Delta \varepsilon_{ij} &= \frac{1}{2}(\Delta u_{i,j} + \Delta u_{j,i}) = B_{ijk} \Delta u_k, \\ \Delta \sigma_{ij}^e &= \Delta \sigma_{ij} - \Delta \sigma_{ij}^c = D_{ijkl}(\Delta \varepsilon_{kl} - \Delta \varepsilon_{kl}^c), \end{aligned} \right\} \quad (7)$$

where $\Delta \sigma_{ij}$, $\Delta \varepsilon_{ij}$ and Δu_i are incremental stress, strain and deformation, respectively, during the specified time increment, Δt . The superscripts e and c denote the elastic and creep parts, respectively. In the above, the incremental creep strain $\Delta \varepsilon_{ij}^c$ is prescribed by the multi-axial constitutive equation of elasto-creep model

$$\Delta \varepsilon_{ij}^c = \frac{3}{2} \frac{\Delta \bar{\varepsilon}^c}{\bar{\sigma}} S_{ij}, \quad (8)$$

where $\Delta \varepsilon^c$ is defined by $\Delta \bar{\varepsilon}^c \Delta t$ for the uniaxial creep rate ($\Delta \bar{\varepsilon}^c$), the equivalent stress ($\bar{\sigma}$) and the deviatoric stress (S_{ij}). Only $\Delta \bar{\varepsilon}^c$ is provided by the uniaxial creep testing for the constitutive matrix material.

The variational equation equivalent to both the governing equations (7) and the natural boundary conditions on the surface S_σ , is given by

$$\int_V v_j B_{lmj} D_{lmpq} B_{pqi} \Delta u_i \, dV = \int_V v_j B_{pqj} \Delta \sigma_{pq}^c \, dV + \int_{S_\sigma} v_j \Delta \bar{T}_j \, dS \quad \text{for } v_j \in H(V) \quad (9a)$$

or

$$A(\Delta u_i, v_j) = F(v_j) \quad \text{for } v_j \in H(V). \quad (9b)$$

Substituting Eq. (2) into (9) and arranging the equations on the basis of the homogenization theory, Eq. (9) provides a simultaneous system of variational equations for macro- and micro-models. That is, the variational equation in the macro-model is given by

$$\int_V v_j B_{lmj}^x D_{lmpq}^H B_{pqi}^x \Delta u_i^0 \, dV = \int_V v_j B_{lmj}^x \Delta \sigma_{lm}^H \, dV + \int_{S_\sigma} v_j \Delta \bar{T}_j \, dS \quad \text{for } v_j \in H(V), \quad (10)$$

where B_{ijk}^x denotes B -operator in the x -coordinates, and, the homogenized stiffness D_{ijkl}^H and incremental creep stress $\Delta \sigma_{ij}^H$ are, respectively, given by

$$\left(D_{ijkl}^H = \frac{1}{|Y|} \int_Y D_{ijkl} - D_{ijpq} \frac{\partial \chi_p^{kl}}{\partial y_q} \right) dY, \quad (11)$$

$$\Delta \sigma_{ij}^H = \frac{1}{|Y|} \int_Y (\Delta \sigma_{ij}^c - D_{ijkl} B_{klj}^y \psi_j) dY. \quad (12)$$

While, since a solution Δu^1 for the micro-model can be expressed by $\Delta u_i^1 = -\chi_i^{(kl)} \Delta \varepsilon_{kl}^x(u^0) + \phi_i(x, y)$, its variational equations are given by

$$\int_Y v_j B_{lmj}^y D_{lmpq} B_{pqi}^y \chi_i \, dY = \int_Y v_j B_{lmj}^y D_{lmpq} \bar{\varepsilon}_{pq} \, dY \quad \text{for } v_j \in H(Y), \quad (13)$$

where $\bar{\varepsilon}_{pq}$ is a prescribed uniform strain in the unit cell, and, B_{ijk}^y the B -operator in the y -coordinates, and

$$\int_Y v_j B_{lmj}^y D_{lmpq} B_{pqi}^y \psi_i \, dY = \int_Y v_j B_{lmj}^y \Delta \sigma_{lm}^c \, dY + \int_{S_\sigma} v_j \Delta \gamma n_j \, dS \quad \text{for } v_j \in H(Y), \quad (14)$$

where $\Delta \gamma$ is the prescribed surface tension increment on the surface of porosity with the normal directional vector n_i . Simultaneous solution of Eqs. (10), (13) and (14) determines the total deformation, the accumulated strain and current stress state at the time (t) together with the estimate of microstructure by D_{ijkl}^H . To be noted, the macroscopic, geometric configuration (V) and the unit cell configuration (Y) can change themselves with strong dependency on the process transients and shrinkage of local porosity.

3.3. Physical coupling among three field variables

Each modeling field can be designed to have coupling among related fields at the specified level in the hierarchical structure. In the present macro–micro modeling, three types of coupling are

considered: elasto-creep model vs. thermal conduction model, thermal effect on the diffusion process and diffusion effect on the elastic response. In the first coupling, the creep strain rate is determined as a function of temperature, while temperature distribution is considered in the deformed material domain. This coupling is considered in the micro-models. In the second coupling, the thermal dependency of diffusion coefficient is directly considered in the micro-model. In the third coupling, the elastic properties in the micro-model is assumed to be dependent on the mass fraction of diffusing elements.

4. Numerical examples

Validity and effectiveness of the present method is demonstrated through the following numerical examples.

4.1. Numerical validation of the present method

A two-dimensional elastic problem was employed here to utilize the analytical solution by the micromechanics [10] for description of the convergence behavior of the present solution. Hassani et al. [8] solved analytically the equivalent stiffness for a two-dimensional cell with a square cavity as depicted in Fig. 4. The full-dense material is assumed to be in isotropic elasticity: $D_{1111} = D_{2222} = 30$, $D_{1122} = 10$ and $D_{1212} = 10$. At the presence of the square cavity located at the center in the unit-cell, the equivalent stiffness D_{ijkl}^H becomes anisotropic; due to the local stress distribution in the uniformly strained unit cell, each modulus in D_{ijkl}^H is further reduced from the original value in D_{ijkl} . In the present method, the unit cell in Fig. 4 was subdivided by six-node triangular elements. For each prescribed uniform strain state, the local stress distribution can be determined by solving Eqs. (13) and (14). Then, every component of D_{ijkl}^H is deduced by using Eq. (11) from the calculated deformations and stresses.

Table 2 compared the calculated components in D_{ijkl}^H with the Hassani's analytical solutions [8] and the Kikuchi's data [4]. In the present computation, the number of elements is 1946 and the number of nodes, 4092. Under this fine mesh model, the present solutions of D_{1111} , D_{2222} , D_{1122} and D_{1212} all converge to the analytical ones with sufficient accuracy. As partially discussed in [8], the Kikuchi's approach provided the upper bound of the analytical solution, while the present

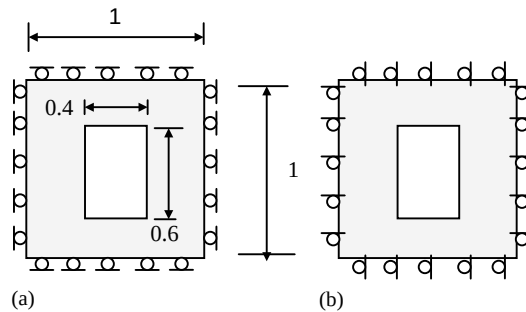


Fig. 4. Unit cell in the two-dimensional elasticity with the square cavity.

Table 2

Comparison of the present solution with the analytical solution and the Kikuchi's data

Solution	D_{1111}	D_{1122}	D_{2222}	D_{1212}
Kikuchi	13.015	3.241	17.552	2.78
Hassani	12.839	3.124	17.422	2.648
This method	12.826	3.12445	17.4083	2.6348

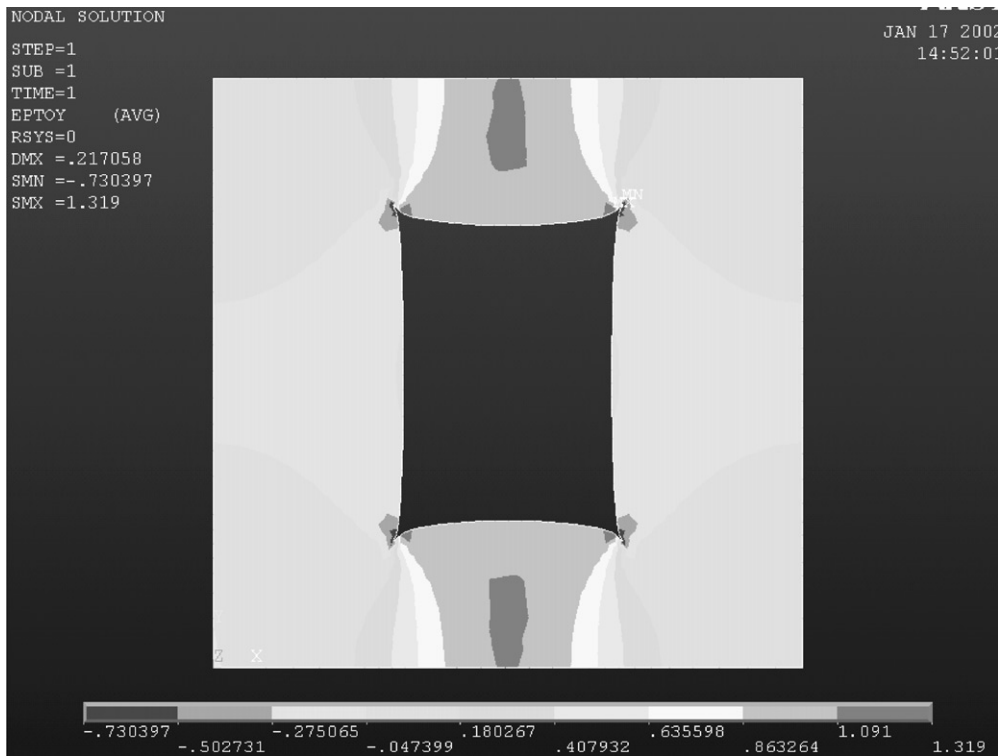


Fig. 5. Normal stress distribution in the unit cell when the normal strain is uniformly prescribed.

solution converges to the analytical one from the lower bound. As had already been noticed in [13], this might be partially because of the stress concentration around the cavity in the unit cell. As shown in Fig. 5, the normal stress state significantly changes at the vicinity around each corner of a square cavity. Hence, without adequate selection of finite element subdivision and scheme, sufficient convergence might never be attained in computation of the equivalent stiffness.

4.2. Hot deformation in sintering without pressure

In the conventional sintering, the isolated pores in the powder compact are closed by the surface tension at the elevated temperature. In the case when the pore size distributes in the compact,

Table 3
Fundamental data for hot deformation and sintering analysis

Uniaxial creep strain rate ^a	$\dot{\epsilon}^c = 16\alpha\beta\Omega D \exp(-U/RT)\sigma/(\pi l^2 kT)$
Parameters	Material constants: $\alpha = 1$, $\beta = 1$ Diffusion coefficient: $D = 1.45 \times 10^{-13} \text{ m}^2/\text{s}$ Atomic volume: $\Omega = 1.0 \times 10^{-29} \text{ m}^3$ Edge length of a grain: $l = 1 \text{ }\mu\text{m}$ k : Boltzmann coefficient U : Activation energy T : Temperature
Elastic properties	Young's modulus: $E = 130 \text{ GPa}$ Poisson's ratio: $\nu = 0.343$
Surface traction	$\gamma = 1.72 \text{ J/m}^2$

^aCopper powders are employed as a reference material. This functional form stands on the body-diffusion mechanism in sintering.

macroscopic shrinkage in geometry never takes place uniformly, resulting in the distortion of a sintered product. Table 3 summarized the computational conditions for sintering analysis. Although those material properties listed in this table were cited for the copper, various kinds of creep laws can be installed into the present system.

In Fig. 6, the pore size distribution was modeled by using the different unit cells, and the variation of geometry and stress distribution was simulated by the present method. Local shrinkage is strongly dependent on the pore size, so that the sintering strain and stress distribute in the sintered product. In the present case, since more porous sections were easy to be sintered, a product was totally bent to the upper direction and geometric irregularity was frozen in the final shape as reported in experiment [3].

4.3. Sintering in hot pressing

Hot pressing is a typical P/M processing to fabricate the dense sintered compact. Through various experiments, temperature and pressure schedules in processing are important to make high densification. In this example, porosity size distribution is also considered by using the different unit cells as illustrated in Fig. 7. Unit-cell models from “A” to “C” in Fig. 7 have the same average porosity density in area, but local size distribution is assumed to be different. Coupling between the thermal distribution and the hot deformation is also considered to discuss the effect of pressurizing in hot pressing on the sintering behavior.

In the absence of isostatic pressure, since fine porosities are easy to be closed by surface tension, the product was forced to be bent upward even in the uniform temperature condition. This might be because local shrinkage is exaggerated in section “A” where finer porosity distributes. In fact, as shown in Fig. 8(a), porous materials with finer porosity undergo larger sintering strains. In case of hot pressing, the externally applied stress effect is superposed on the above sintering stress state. Figs. 8(b) and (c) show the macroscopic deformation and stress state, and, the microscopic shrinkage

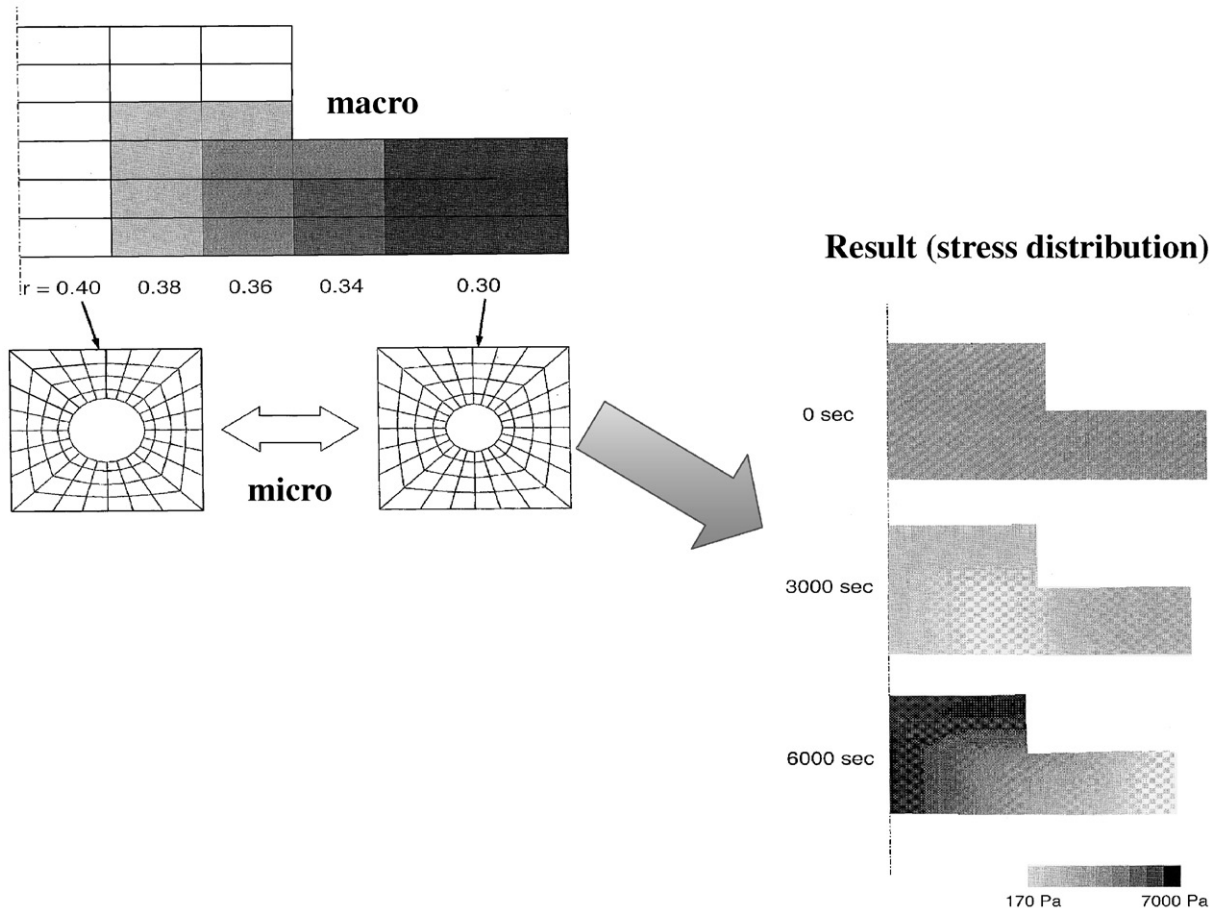


Fig. 6. Hot deformation of powder compact with the porosity distribution during sintering.

during sintering, respectively. No geometric distortion was generated since the externally applied stress has more dominant influence on the activation of sintering. To be noticed in comparison between Figs. 8(a) and (c), local shrinkage was enhanced by this application of external pressure.

4.4. Sintering during hiping process

Hot isostatic pressing or hiping process is frequently utilized for sintering ceramic materials to full density. In this process, the starting porous materials are thought to be gradually sintered to the state, where isolated pores are only left in dense materials, and these pores are absolutely closed in high dense compact. Fig. 9(a) illustrates the hiping experimental condition of austenitic stainless steel (SUS316L) powders with the average size of 50 μm . Table 4 lists the experimentally measured material properties and constitutive equations for SUS316L bulk materials. Starting from the initial geometry with uniform porosity distribution, both hiping experiment and simulation trace the prescribed thermal and pressurizing schedules in Fig. 9(a). Fig. 9(b) compares the volumetric strain

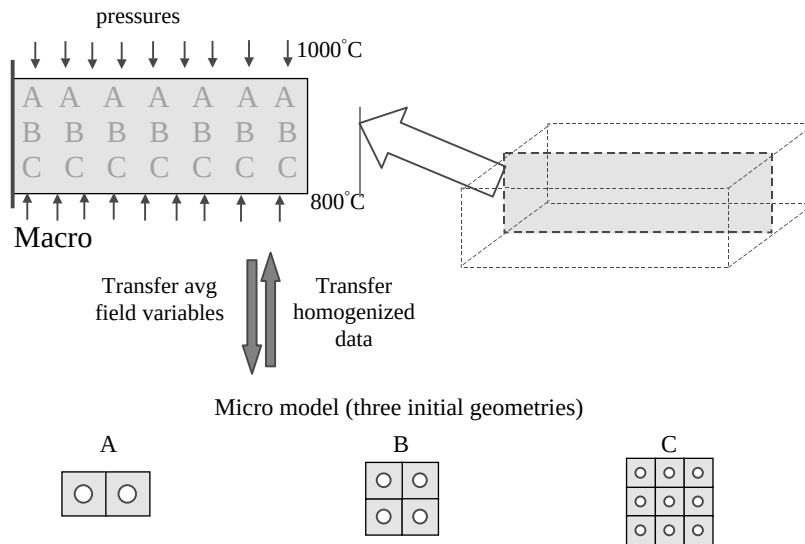


Fig. 7. Unit-cell modeling to consider the local porosity distribution with the constant average porosity.

Table 4
Computational conditions for hipping process simulation

Materials property	Functional form
Young's modulus ^a (MPa)	$19400 - 81.4T$ for $T < 973$ K
Poisson's ratio	0.3
Thermal conductivity (W/m K)	$13.651 + 0.01434T$
Specific heat (J/kg K)	$465.45 + 0.21045T + 8.6641 \times 10^{-7}T^2$

^a Above 973 K, Young's modulus is supposed to decrease monotonically to zero with T up to the melting temperature (1648 K).

rate and the average relative density between experimental and simulated results, respectively. The present modeling can predict the time history of volumetric strain rate with fairly good accuracy. This might be because geometric sintering strain rate experimentally measured is approximately governed by local shrinkage rate of a closed pore. On the other hand, gradual densification observed in experiment revealed that heterogeneous shrinkage took place in the macroscopic sintering process.

4.5. Coupling of deformation model with diffusion process

Mass transportation in the diffusion process must be taken into account in the microstructure evolution. Coupling between deformation and diffusion models is considered to investigate the effect of constitutive element redistribution during diffusion on the variation of equivalent elastic properties. Mixture of pure nickel and copper was considered as a starting material, and, mutual diffusion was

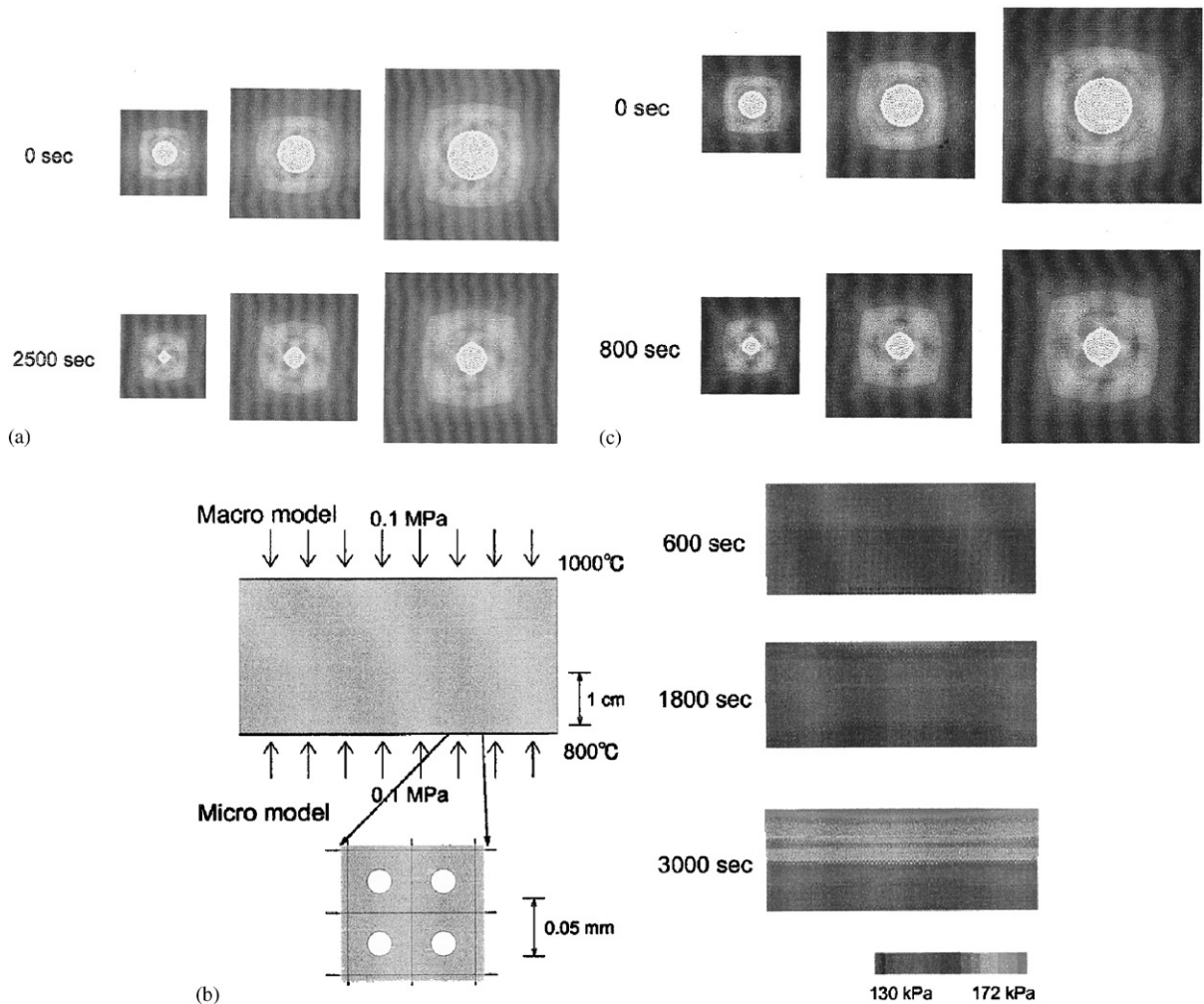


Fig. 8. (a) Local shrinkage behavior observed in the unit cells with different initial porosity size in the absence of the externally applied pressure. (b) Macroscopic geometry change during hot pressing. (c) Local shrinkage behavior observed in the unit cells with different initial porosity size in the presence of the externally applied pressure.

assumed to take place between both elements. As shown in Fig. 10(a), both elements are mixed with time through the mutual diffusion process. In parallel with that, the homogenized stiffness D_{ijkl}^H also varies with the diffusion time. Fig. 10(b) depicts a typical increase of D_{1111}^H component in D_{ijkl}^H with diffusion time.

5. Discussion

In the conventional nonlinear analysis, construction of constitutive equations to represent actual materials nonlinearity is one thing but theoretical modeling is another. Hence, when using the

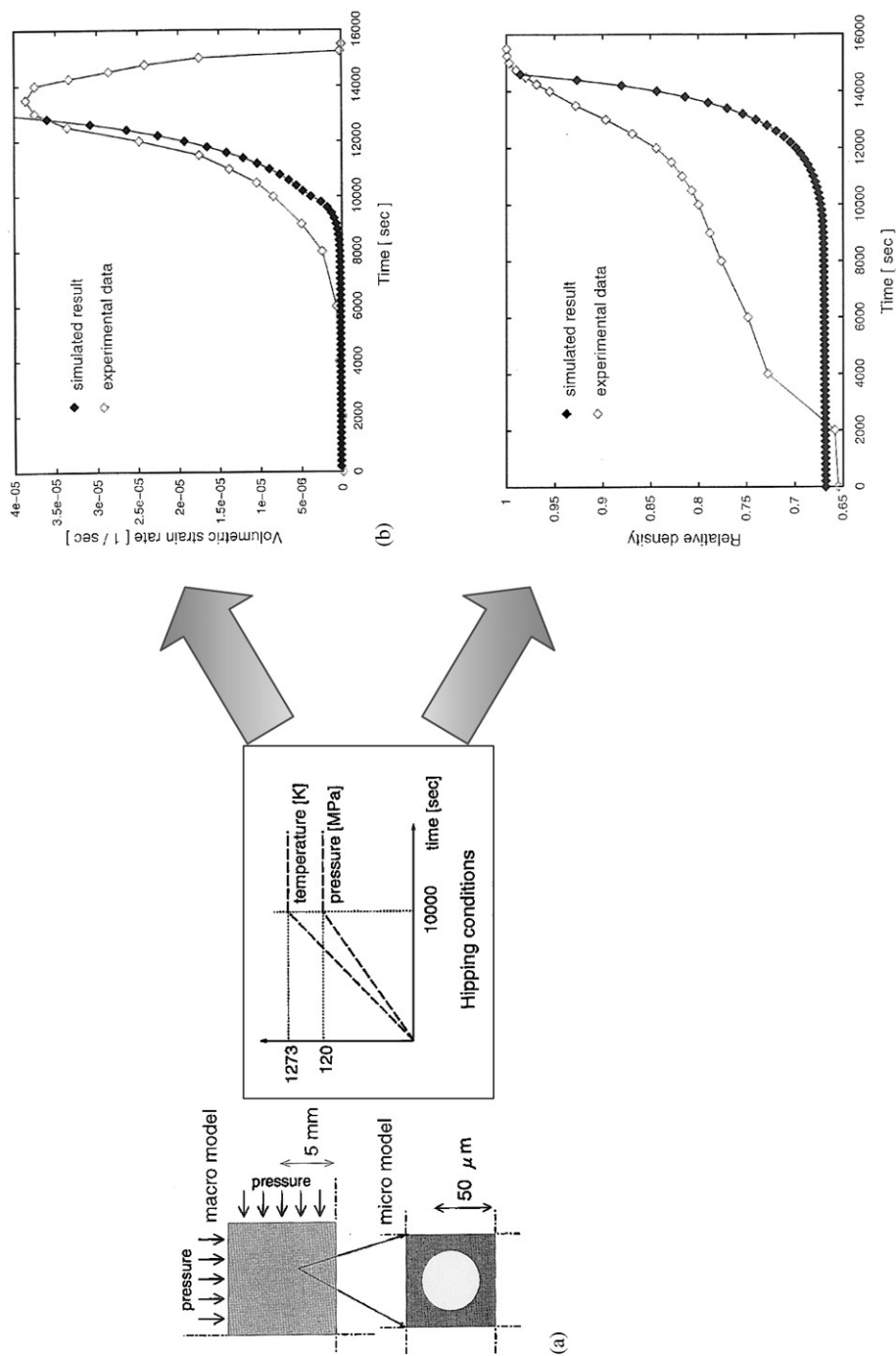


Fig. 9. (a) Specification of unit cell and thermal/loading transients to be used in simulation. (b) Comparison of experimental and calculated time histories of volumetric strain rate and relative density.

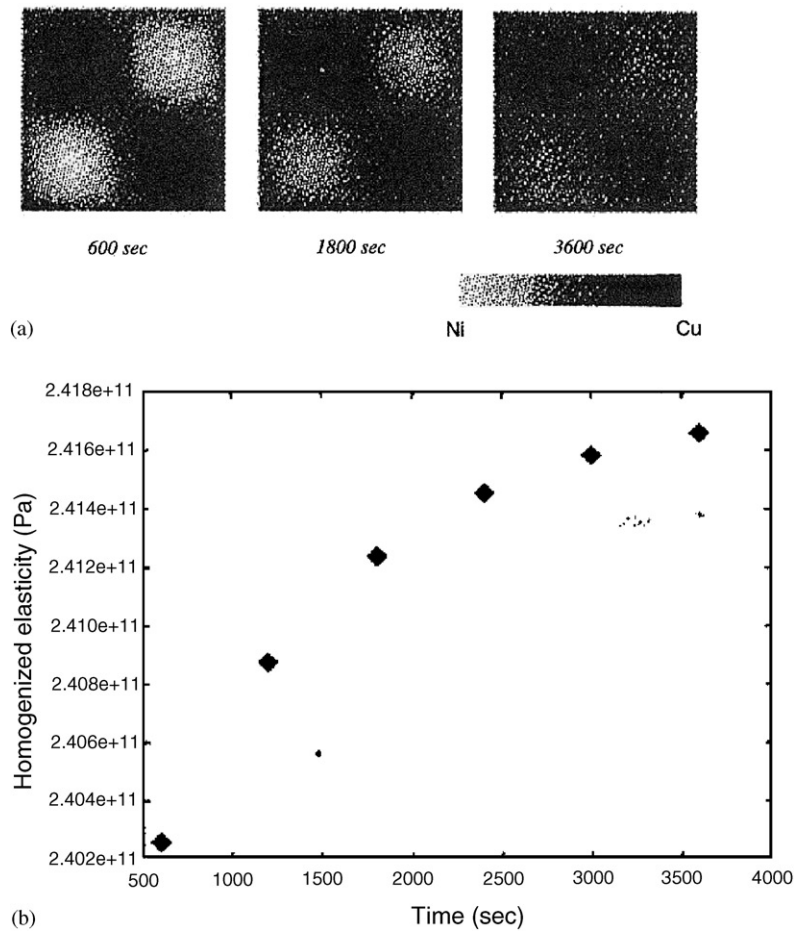


Fig. 10. (a) Redistribution of constitutive elements with the diffusion time. (b) Variation of D_{111}^H component in the homogenized stiffness D_{ijkl}^H with the diffusion time.

nonlinear finite element method for simulations, complex constitutive equations must be obtained to explain the targeting nonlinear phenomena physically. While, the microstructure information, which had been obtained through precise observation, is difficult to utilize in the above nonlinear simulation. Aiming for more accurate nonlinear analysis, only macroscopic data by experiments is insufficient as an essential key to determine the quality of simulation. Promising, quantitative simulation must be equipped with prediction of microstructure change at the elevated temperature. The present coupled, multi-level modeling is the first prototype for this kind of simulation.

As discussed in the above, the homogenized stiffness becomes a measure to mechanically evaluate the microstructure evolution. During sintering the powder compact, the equivalent elastic stiffness increases itself with gradual reduction of porosities with time. Fig. 11 showed the comparison of Young's modulus between the experimental and calculated results. In experiment, Young's modulus was evaluated from the measured lateral and shear wave velocities of each sintered SUS304 powder

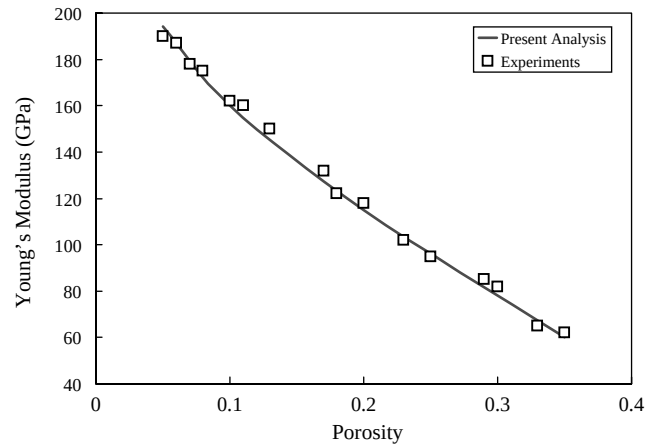


Fig. 11. Comparison of the evolution of Young's modulus during sintering between the experimental and calculated results.

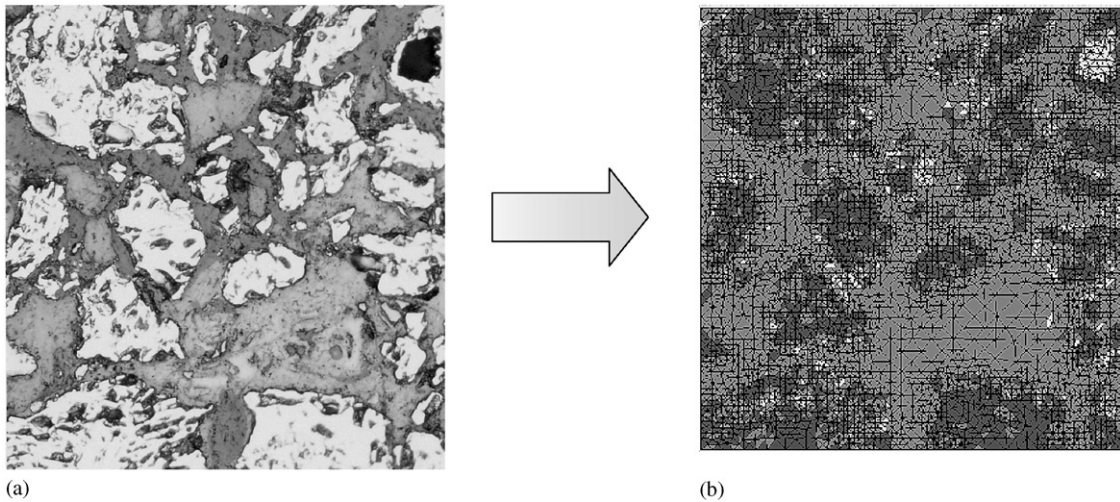


Fig. 12. Conversion of a microstructure image obtained by optical microscope to a mathematical model for the finite element analysis: (a) mixture of iron ore and coal with porosities, and (b) finite element mesh model with each material property allocated to element.

compact with different porosity by the ultrasonic method. In the present computation, the unit cell was set up to the initial powder compact with the porosity of 40%. Young's modulus was deduced from the calculated stiffness matrix D_{ijkl}^H by the time marching simulation in the present method. Good agreement between two in Fig. 11 reveals that the homogenized stiffness should be equivalent to actual elastic properties of sintered materials.

In the present approach, the microstructure observation and analysis reflects on the coupling model at the microscopic level and on the unit cell to be employed. In the above numerical examples, the unit-cell models were selected to correspond to the powder particle configuration or the initial particle

assembly. Through recent our work, however, actual microstructure observed by optical microscope or scanning electron microscope (SEM) can be image processed and converted to a mathematical model with a unit cell. Typical example was shown in Fig. 12. Using the computer-aided scanner and utilizing the image processor combined with automatic mesh generator, the microstructure information for a mixture of iron ore and coal with porosities can be converted to a mathematical model for finite element analysis [2]. The unit cell size can be also determined by computing the homogenized stiffness; an optimum cell size is just corresponding to the convergent value of the calculated equivalent stiffness.

6. Conclusion

Hot deformation during the sintering process was selected in the present method as a target for coupled, macro–micro modeling. In this theoretical frame, grain growth or microstructure evolution, which has been described by the discrete modeling like the MC method, can be also formulated by using the nonlinear diffusion model [11]. Effective diffusion coefficients needed for the above formulation must be determined by physical conversion of the simulated time history of mass transportation by MC. The most favorite feature to this approach lies in the capability to consider the chemical reaction as a nonlinear term. Various microstructure changes with chemical reaction taking place in the reactive sintering or the solid-state synthesis, can be dealt with by this method.

Coupling among the stress/deformation model, the thermal transient model and the transportation of chemical potential, is also necessary as an extension of the present coupled macro–micro modeling. Phase transformation often accompanies with significant volumetric change, resulting in large strains or fracture in hot deformation. Time history of temperature is directly affected by phase transformation. Through this new coupled, multi-level modeling, qualitative understanding of mechano-chemical interactions can be changed into quantitative description by theoretical simulation.

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