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Three-scale finite element analysis of heterogeneous media by asymptotic homogenization and mesh superposition methods

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Abstract

This paper studies a three-scale computational method that simultaneously considers the microstructure of heterogeneous materials, the macroscopic component, and the fracture origin such as interface or crack. The synergetic application of the asymptotic homogenization and mesh superposition methods to problems with strong scale mixing is emphasized. The scale gap between the microstructure and the component is very large, but the fracture origin is at the middle scale between them. The overall behavior is analyzed by means of the homogenization of the heterogeneity expressed by the unit cell model, while the fracture origin is modeled directly with the microscopic heterogeneity by another microscopic mesh. The microscopic mesh is superposed onto the macroscopic mesh. This mesh superposition method can analyze the non-periodic microscopic stress at the crack tip under a non-uniform macroscopic strain field with high gradient. Hence, the present three-scale method can accurately focus on the behaviors at arbitrary scale differently from the conventional hierarchical model. A demonstrative example of porous thin film on a substrate with an interface crack was solved and the microscopic stress was analyzed at the crack tip considering the random dispersion of pores and the high gradient of macroscopic strain field. To solve the large-scale 3D problem with approximately 80,000 solid elements, a renumbering technique and the out-of-core skyline solver was employed.

Keywords: Multi-scale analysis; Finite element method; Mesh superposition; Homogenization; 3D analysis; Microstructure; Heterogeneity; Interface crack

1. Introduction

The design and control of the hierarchical structural elements ranging from atomic or nanoscale to microscale is supposed to be a promising approach toward the research and development of various advanced materials such as advanced composite materials, polycrystalline materials, and porous materials.

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Therefore, there is a growing need for multi-scale computational methods to study the correlation between the microstructure and the macroscopic properties.

This paper aims at solving the mechanical behaviors of heterogeneous materials considering simultaneously the microstructure, the macroscopic component, and the fracture origin such as interface or crack. The scale gap between the microstructure and the component is very large, but the fracture origin is at the middle scale between them. Consequently, we want to focus on the behaviors at various scales depending on the dimension of the fracture origin. The conventional hierarchical model is not applicable to this problem. When analyzing the microscopic behaviors at the macroscopic crack tip, the multi-scale method has to solve the microscopic problems under high gradient of macroscopic stress/strain field.

The asymptotic homogenization method coupled with the finite element method (FEM) has been supposed to be the most effective tool especially for the analysis of the microstructural effect on the overall properties of the above-mentioned heterogeneous media. This theory was first developed during the 1970s and 1980s (Lions, 1981) and was applied to textile composite materials by Guedes and Kikuchi (1990). During the last decade this theory has been the subject of several intensive researches, including the exploitation of non-linear applications (Ghosh et al., 1996; Takano et al., 2000a, Terada and Kikuchi, 2001), studies on high-speed and practical modeling and numerical algorithms (Shephard et al., 1995; Fish et al., 1997; Moulinec and Suquet, 1998), and the validation by experimental facts (Takano et al., 2001a, 2003a). The reason why this method is not applicable to problems studied in this paper is briefly recalled below.

A microscopic unit cell model is used that represents the heterogeneous microstructure with periodicity condition. If the microscopic crack is considered, we have to assume that the unit cell model with a crack is repeated. In other words, a locally existing microscopic crack cannot be analyzed using this theory. Basically, material with a local crack cannot be replaced by the equivalent homogenized property, because the volume averaging depends on the dimension of the representative volume element (RVE). Caiazzo and Costanzo (2001) derived the equivalent constitutive model for laminated composite materials with cracks. However, in this case, the correlation between the cracks and the heterogeneous fibers' arrangement has not been taken into account. We can only apply the damage mechanics approach to such problems (Takano et al., 1999; Fish and Yu, 2002). More importantly, the periodicity is assumed not only for the geometrical architecture but also for the physical quantities such as displacements, strains and stresses (Takano et al., 2000a, 2001a). To this end, microscopic analysis under high gradient of macroscopic fields may fail if the asymptotic homogenization method is used. This problem was detected at an early stage (Fish et al., 1997; Lee et al., 1999) but has not yet been resolved.

The higher-order theory and the non-local approach can provide a solution to this problem (Benallal and Tvergaad, 1995; Triantafyllidis and Bardenhagen, 1996; Schraad and Triantafyllidis, 1997; Knockaert and Doghri, 1999). Although the second-order theory can consider the non-linear distribution of the macroscopic strain in the microscopic region under analysis, the gradient of the macroscopic strain is modeled to be constant in this theory. Since the real microscopic region has finite and various dimensions, it may lead to a critical error especially when a fracture origin such as a crack is considered.

Instead, together with the homogenization method, Fish and Wagiman (1993), Lee et al. (1999), and Ghosh et al. (2001) used another microscopic model that directly expresses the microscopic heterogeneity of the microscopic region to be analyzed. Lee et al. (1999) and Ghosh et al. (2001) used the microscopic finite element mesh in a type of hierarchical model with a transition element. The transition element connects the microscopic heterogeneous model and the homogenized model. Furthermore, Fish and Wagiman (1993) superimposed the microscopic model onto the homogenized model. This finite element mesh superposition method was originally presented by Fish (1992) under the name of s-version FEM, in a series of studies on the adaptive FEM. The s-version FEM and other similar methods were applied to the modeling of smart materials and structures (Robbins Jr. and Reddy, 1996), crack propagation problems (Rashid, 1998), and elasto-plastic problems (Nakasumi et al., 2002). The above applications are limited to homogeneous materials, such as the crack propagation in metals. The authors have also applied this method, as the mesh refinement method, in the modeling of textile composites (Takano et al., 1999).

Since the mesh superposition method can be applied to heterogeneous media the authors have studied its applicability to various advanced materials and its numerical accuracy. Till date, the accuracy and efficiency in modeling have been confirmed in the 2D analysis for the locally existing inclusion/void (Takano et al., 2000b), microscopic crack behavior affected by reinforcing fibers (Takano et al., 2001b), and interface crack behavior affected by pores (Takano et al., 2003b).

After these preliminary studies focused on the implementation and numerical accuracy of the mesh superposition method, this paper presents the synergetic application of the mesh superposition and homogenization methods for three-scale 3D analysis considering simultaneously the microscopic heterogeneity, crack, and macroscopic component. It should be noted that the dimensions of crack are set to be between the dimensions of the microstructure and the macroscopic component. Also the robust and large-scale equation solver for the 3D mesh superposition method is described. A numerical example of porous thin film with a crack is discussed.

2. Framework of three-scale stress analysis and computational methods

In this study on multi-scale computational methods, the microstructure of advanced materials is considered to be in the order of nano- to micrometers. The dimension of the component ranges from 100 mm to 1 m. Consequently, the scale gap between the microstructure and macroscopic component is more than one thousand as shown in Fig. 1. Such a large gap can be correlated by means of the homogenization method. The formulation of this method has been discussed in many papers mentioned in Section 1.

One of the merits of the multi-scale analysis is the calculation of microscopic behaviors. An important issue is that, in the design of materials and components, the microscopic stress evaluation is required at the crack tip, interface or in the local area where macroscopic stress is concentrated. Such fracture origin is usually in the order of 10 μm to 1 mm, ranging between the microstructure and the macroscopic component. The correlation between the fracture origin and the microstructure must be considered. Although the scale gap is approximately 10–100, conventional and direct modeling is not applicable because 3D modeling requires huge data in the range of 10^3–100^3. We have to discuss the complex scale mixing and solve the precise behavior at arbitrary scale depending on the dimension of the fracture origin. Hence, the finite element mesh superposition method is employed to model such a fracture origin. Fig. 2 illustrates the

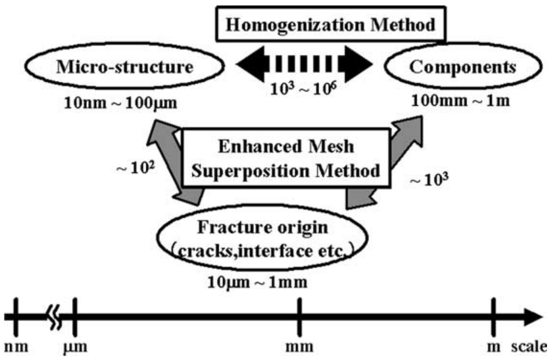

Fig. 1. Framework of three-scale stress analysis.

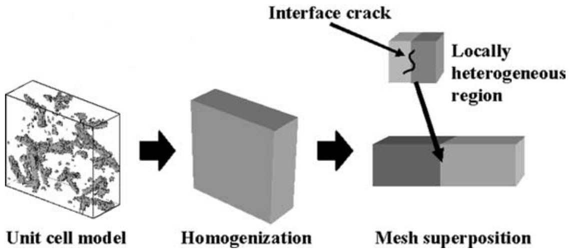

Fig. 2. Multi-scale modeling strategy.

proposed multi-scale modeling strategy using both the homogenization and the mesh superposition methods. One can define arbitrary the microscopic region to be studied precisely considering both the fracture origin and the microscopic heterogeneity influenced by the macroscopic boundary conditions.

Previous studies (Takano et al., 1999; Guedes and Kikuchi, 1990; Ladeveze, 1995) have proposed a hierarchical three-scale modeling strategy for the fiber reinforced composite materials, where single fiber is defined as microscale, woven or knitted architecture is defined as mesoscale, and the component is defined as macroscale. The mesostructure is defined by the periodic assembly of microstructures and becomes a unit cell in the macrostructure. In other words, the mesoscale is uniquely defined for the target materials. Therefore, the fracture origin studied in this study cannot be considered as the mesoscale in the conventional multi-scale framework. On the other hand, in this paper, a different framework of the three-scale problem has been studied and the finite element mesh superposition method has been used to bridge the fracture origin and the other two scales as shown in Fig. 1.

Attention should be paid to the assumption of the periodicity of the microstructure in the analysis of the microscopic behavior under a large macroscopic stress/strain gradient to consider the fracture origin as the third scale. Fig. 3 illustrates the microscopic situation under a non-uniform macroscopic field near the interface crack tip. (Refer to Fig. 1 from the previous paper (Takano et al., 2000a) for comparison.) If we remind that the microstructure of various advanced materials has a finite dimension in reality, the macroscopic stress/strain gradient in the microstructure can be illustrated as in Fig. 4. In this figure, u^0 denotes the macroscopic displacement. The macroscopic strain gradient is strongly non-linear in the microstructure with a finite dimension. The higher-order theory can only consider a case that the strain gradient is constant in the microstructure. On the other hand, the finite element mesh superposition method is applicable even if the strain gradient is high and not constant.

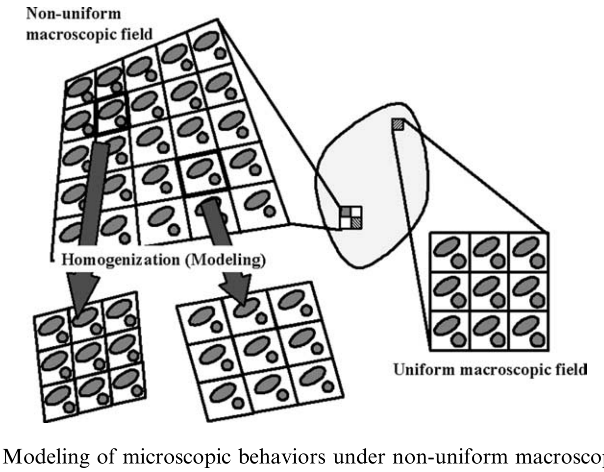

Fig. 3. Modeling of microscopic behaviors under non-uniform macroscopic field.

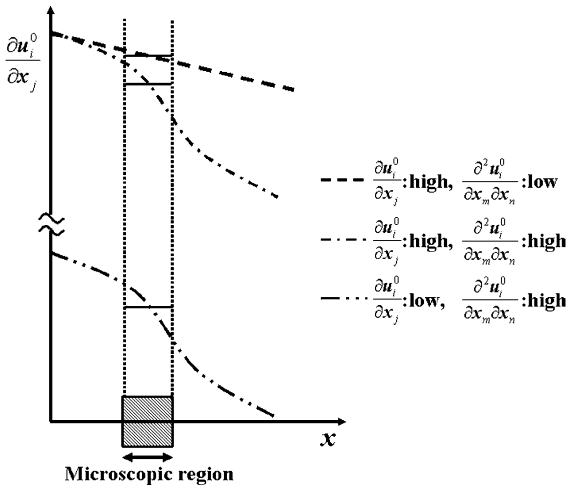

Fig. 4. Non-linear macroscopic strain field with high gradient.

3. Finite element mesh superposition method

The finite element mesh superposition method (Fish, 1992; Fish and Wagiman, 1993) uses two independent meshes. One of them is the macroscopic mesh that uses the homogenized material model reflecting microscopic heterogeneity. The other one is the microscopic mesh that is arbitrarily superimposed onto the macroscopic mesh, without taking care of matching nodes. The microscopic heterogeneity is modeled directly on the microscopic mesh and local heterogeneity such as void, inclusion, crack, interface, etc. (Takano et al., 2000b, 2001b, 2003b).

As shown in Fig. 5, Ω is the overall region and Γ is its boundary. The local region, onto which the microscopic mesh is superimposed, is Ω^L. Ω^G is defined as $\Omega \setminus \Omega^L$. Γ^{GL} is the boundary between Ω^G and Ω^L. The external force $\boldsymbol{p}$ is supposed to be applied to the macroscopic boundary only and is not applied directly to the microscopic mesh Ω^L in this paper. Hereafter, the suffix G denotes the global (macroscopic) quantity and the suffix L denotes the local (microscopic) quantity.

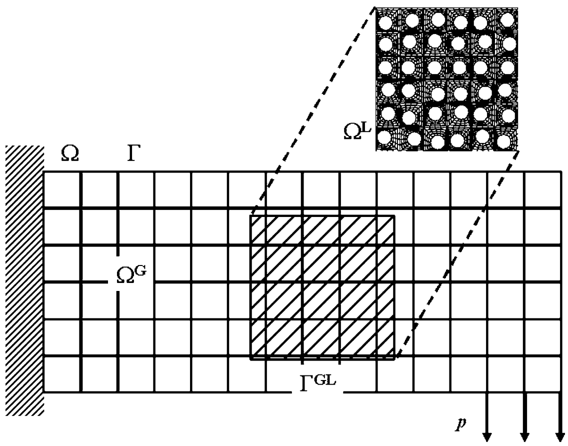

Fig. 5. Setting of macroscopic domain and microscopic region.

The displacement is written as follows:

$$\boldsymbol{u} = \begin{cases} \boldsymbol{u}^{\mathrm{G}} & \text{on } \Omega^{\mathrm{G}},\ \Gamma^{\mathrm{GL}} \\ \boldsymbol{u}^{\mathrm{G}} + \boldsymbol{u}^{\mathrm{L}} & \text{on } \Omega^{\mathrm{L}} \end{cases} \tag{1}$$

It should be noted that the displacement is interpolated in the finite element by the shape function $\boldsymbol{N}$. The mesh superposition method is one of the techniques that allow two meshes with different element sizes. The shape functions of the two meshes connect the macro- and microscopic displacement fields. To retain continuity at the boundary Γ^{GL}, we assume that the following equation holds true.

$$\boldsymbol{u}^{\mathrm{L}} = \boldsymbol{0} \quad \text{on } \Gamma^{\mathrm{GL}} \tag{2}$$

The constitutive equations in each region are written as follows:

$$\boldsymbol{\sigma} = \begin{cases} \boldsymbol{D}^{\mathrm{G}}\boldsymbol{B}^{\mathrm{G}}\boldsymbol{u}^{\mathrm{G}} & \text{on } \Omega^{\mathrm{G}} \\ \boldsymbol{D}^{\mathrm{L}}(\boldsymbol{B}^{\mathrm{G}}\boldsymbol{u}^{\mathrm{G}} + \boldsymbol{B}^{\mathrm{L}}\boldsymbol{u}^{\mathrm{L}}) & \text{on } \Omega^{\mathrm{L}} \end{cases} \tag{3}$$

where $\boldsymbol{D}$ and $\boldsymbol{B}$ denote the elastic stress–strain matrix and strain–displacement matrix. To assure the consistency between the macro- and microscopic governing equations, the homogenized constitutive equation should be predicted by the asymptotic homogenization method accurately for arbitrary complex 3D microstructure architecture. The strain and stress are discontinuous at the boundary Γ^{GL}. The microscopic region Ω^{L} can be arbitrary only if the homogenized constitutive model can be predicted accurately for Ω^{L} in this paper's setting.

Above relations are substituted into the following governing equation.

$$\int_{\Omega} \bar{\boldsymbol{\varepsilon}}^{\mathrm{T}}\boldsymbol{\sigma}\,\mathrm{d}\Omega = \int_{\Gamma} \bar{\boldsymbol{u}}^{\mathrm{T}}\boldsymbol{p}\,\mathrm{d}\Gamma \tag{4}$$

where $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{\varepsilon}}$ are the virtual displacement and strain, respectively. Note again that, in this problem setting in Fig. 5, the external force is applied only to the macroscopic mesh. However, it is not the limitation of the mesh superposition method, and the external force, body force, and thermal stress can be considered if needed (Fish, 1992; Takano et al., 2003b).

$$\begin{bmatrix} \boldsymbol{K}^{\mathrm{G}} & \boldsymbol{K}^{\mathrm{GL}} \\ (\boldsymbol{K}^{\mathrm{GL}})^{\mathrm{T}} & \boldsymbol{K}^{\mathrm{L}} \end{bmatrix} \begin{Bmatrix} \boldsymbol{u}^{\mathrm{G}} \\ \boldsymbol{u}^{\mathrm{L}} \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{f} \\ \boldsymbol{0} \end{Bmatrix} \tag{5}$$

where

$$\boldsymbol{K}^{\mathrm{G}} = \int_{\Omega^{\mathrm{G}}} (\boldsymbol{B}^{\mathrm{G}})^{\mathrm{T}}\boldsymbol{D}^{\mathrm{G}}\boldsymbol{B}^{\mathrm{G}}\,\mathrm{d}\Omega^{\mathrm{G}} + \int_{\Omega^{\mathrm{L}}} (\boldsymbol{B}^{\mathrm{G}})^{\mathrm{T}}\boldsymbol{D}^{\mathrm{L}}\boldsymbol{B}^{\mathrm{G}}\,\mathrm{d}\Omega^{\mathrm{L}} \tag{6}$$

$$\boldsymbol{K}^{\mathrm{GL}} = \int_{\Omega^{\mathrm{L}}} (\boldsymbol{B}^{\mathrm{G}})^{\mathrm{T}}\boldsymbol{D}^{\mathrm{L}}\boldsymbol{B}^{\mathrm{L}}\,\mathrm{d}\Omega^{\mathrm{L}} \tag{7}$$

$$\boldsymbol{K}^{\mathrm{L}} = \int_{\Omega^{\mathrm{L}}} (\boldsymbol{B}^{\mathrm{L}})^{\mathrm{T}}\boldsymbol{D}^{\mathrm{L}}\boldsymbol{B}^{\mathrm{L}}\,\mathrm{d}\Omega^{\mathrm{L}} \tag{8}$$

$$\boldsymbol{f} = \int_{\Gamma} \boldsymbol{N}^{\mathrm{T}}\boldsymbol{p}\,\mathrm{d}\Gamma \tag{9}$$

The stiffness matrices $\boldsymbol{K}^{\mathrm{G}}$ and $\boldsymbol{K}^{\mathrm{L}}$ are calculated using the macroscopic and microscopic meshes, respectively. The interaction between two meshes is expressed by $\boldsymbol{K}^{\mathrm{GL}}$. Hence, the finite element mesh superposition is advantageous over the conventional zooming method (Takano et al., 2003b).

The numerical integration of Eqs. (6) and (7) should be done cautiously because the mesh size of the macro- and microscopic meshes is significantly different when considering the microscopic heterogeneity. We found that Eq. (6) can be approximated by the following simple integration.

$$\boldsymbol{K}^{\mathrm{G}} \approx \int_{\Omega} (\boldsymbol{B}^{\mathrm{G}})^{\mathrm{T}} \boldsymbol{D}^{\mathrm{G}} \boldsymbol{B}^{\mathrm{G}} \, \mathrm{d}\Omega \tag{10}$$

The numerical integration of Eq. (7) has been described in detail in the authors' previous paper (Takano et al., 2001b).

One of the critical issues in applying the mesh superposition method to multi-scale analysis of heterogeneous media is numerical accuracy. In the region where the microscopic mesh is superposed, both the macroscopic and microscopic equilibrium equations are solved simultaneously. Hence, the consistency between the macro- and microscopic equations are essential. That is, the use of the homogenization method is very important to predict the macroscopic properties accurately for arbitrary complex microstructure architecture (Takano et al., 2003a). More importantly, due to the discontinuity in the material models at the boundary Γ^{GL} of the macroscopic model and microscopic model, the margin of error near the boundary Γ^{GL} was not negligible (Takano et al., 2003b). Generally the modeling of heterogeneity with randomness inevitably leads to the numerical error near the boundary region of the microscopic model. There are many successful researches that aimed at predicting the overall properties taking randomness into consideration (Torquato, 1998; Buryachenko et al., 2003). However, the error appears in the analysis and evaluation of the microscopic stress by the homogenization method (Takano et al., 2002). That is also true in the analysis by the mesh superposition method. However, we confirmed that very good accuracy is achieved at the inner region of the microscopic mesh (Takano et al., 2000b, 2001b, 2003b). This factor has been considered in the numerical example in this paper.

Another significant point is the large-scale and robust equation solver. The stiffness matrix in Eq. (5) consists of four blocks, and is not the band matrix due to the interactive term $\boldsymbol{K}^{\mathrm{GL}}$. This implies that the 3D large-scale analysis is very difficult. Therefore, some researchers are attempting to use the preconditioned iterative solver (Shinmura et al., 2002; Okada et al., 2003). Shinmura et al. (2002) found that the convergence is not obtained for some cases. It seems to be related to the difference in mesh size between the macro- and microscopic meshes. It is possible that the discontinuous material model might render the problem ill-conditioned. The same was true in the authors' preliminary studies on a crack problem. On the contrary, the renumbering technique works very well for the block-wise matrix in Eq. (5). Among some renumbering techniques, we employ Reverse-Cuthill–Mckee (RCM) method (Murata et al., 1985). Fig. 6 shows one example of the effect of RCM method. It can be said that renumbering is also effective in cases where multiple microscopic meshes are superimposed simultaneously.

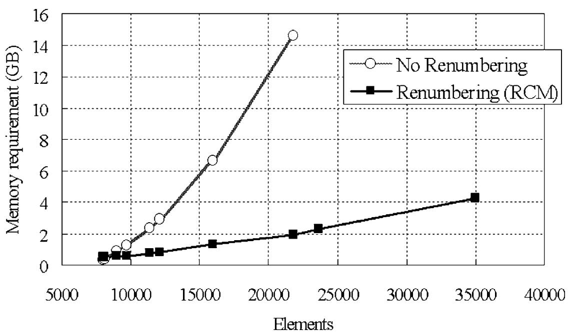

Fig. 6. Comparison of required memory between renumbered and non-renumbered stiffness matrices by mesh superposition method.

4. Numerical example

To demonstrate the effectiveness of the proposed three-scale finite element method, we use a porous thin film coated substrate with an interface crack as shown in Fig. 7. The final goal in this numerical example is to analyze the microscopic stress distribution near the interface crack tip, considering the effects of the microscopic pores that are randomly dispersed under the macroscopic boundary condition. The thin film is supposed to be TiO_2 with randomly dispersed straight pores. The cross section is supposed to be circular with a diameter of 6.2 μm. The porosity ratio is 30%. The substrate is supposed to be SiO_2. The Young's modulus and poisson's ratio of TiO_2 are 228 GPa and 0.27, respectively, whereas those of SiO_2 are 68 GPa and 0.19, respectively. The scale gap between the representative dimensions of the macroscopic component and the microstructure is approximately 330 and that between the interface crack and microstructure is approximately 40, which corresponds to the setting of the three-scale framework shown in Fig. 1. In the analysis by the mesh superposition method, the whole region of this component is Ω and the porous thin film is modeled macroscopically by the equivalent material model predicted by the asymptotic homogenization theory. The microscopic region Ω^L is supposed near the crack tip, where the constitutive materials and pores are directly expressed. By superimposing the microscopic region onto the overall model, the microscopic stress is analyzed under the high gradient of the macroscopic stress/strain field.

The boundary condition shown in Fig. 8 is assumed. Due to the symmetry, half a region is analyzed as the macroscopic model. It is uniformly subdivided by eight noded solid elements. The number of elements and nodes of the macroscopic mesh are 32,000 and 35,771, respectively.

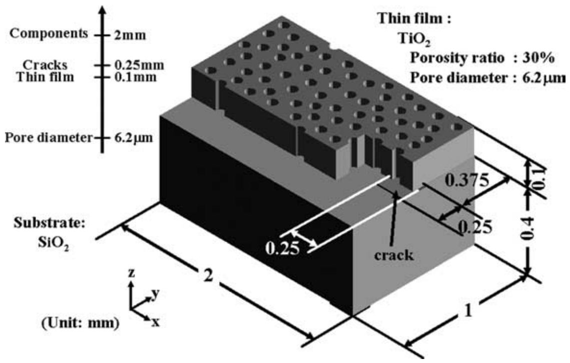

Fig. 7. Porous thin film coated substrate with interface crack.

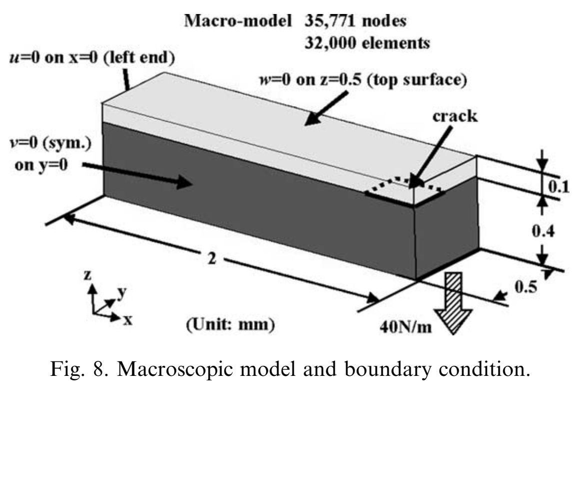

Fig. 8. Macroscopic model and boundary condition.

To analyze the microscopic stress at the interface crack tip considering the random dispersion of pores, the microscopic mesh shown in Fig. 9 is used. The number of solid elements and nodes are 46,080 and 52,385, respectively. Therefore, the total number of elements and nodes equal 78,080 and 88,156, respectively. The total d.o.f. is 264,468. Together with the RCM renumbering, the out-of-core skyline method (block skyline method) (Murata et al., 1985) is used. This solver can solve 3D problem of more than 100,000 elements on a standard personal computer (CPU: Pentium IV) with 60GB hard disk.

The microscopic mesh is superimposed onto the macroscopic mesh at the interface crack tip as shown in Fig. 10. The figure also shows the macroscopic mesh to which a homogenized material model is applied. The difference in element size between the macroscopic and the microscopic meshes is more than 10. The accuracy has been validated for cases with such a large difference in element size (Takano et al., 2001b, 2003b).

The homogenized material properties of porous TiO_2 are predicted by the asymptotic homogenization method using a unit cell model as shown in Fig. 11. Considering that the pores are randomly distributed, only a single pore is modeled in the unit cell for homogenization.

Fig. 12 shows the macroscopic behaviors without using the mesh superposition method. The normal stress σ_z at the crack tip in porous TiO_2 film is plotted in Fig. 12. Since the porous TiO_2 is modeled using equivalent homogenized material in these results, the effect of microscopic heterogeneity has not been observed. The microscopic mesh in Fig. 9 is superimposed on the specified region shown in Fig. 12 with a high gradient of macroscopic stress/strain.

The results of the proposed three-scale analysis by homogenization and mesh superposition methods are shown below. Fig. 13 shows the microscopic stress σ_z. It is to be noted that the boundary region of the microscopic mesh is excluded in this figure because of the numerical error that appears in the boundary region due to the mesh superposition as mentioned in Section 3. However, we mention later that the

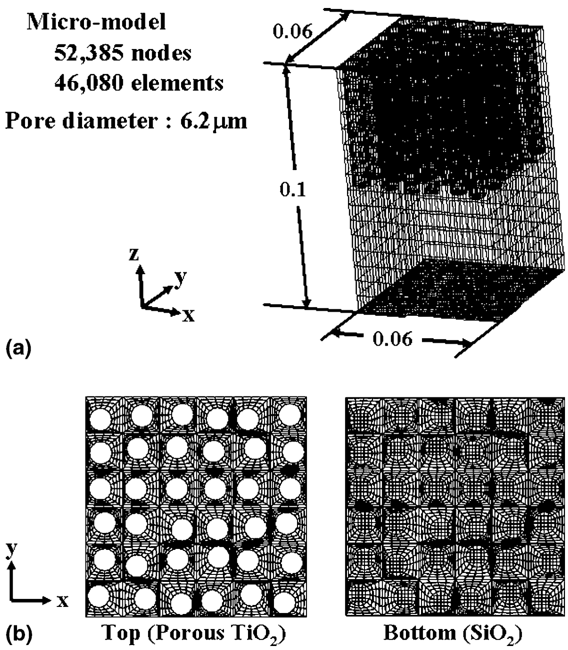

Fig. 9. Microscopic model.

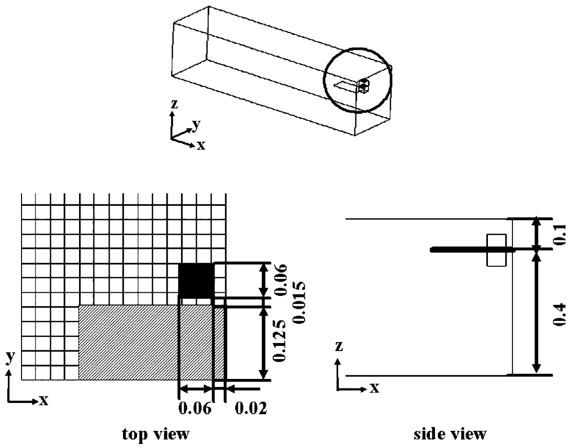

Fig. 10. Superposition of microscopic mesh onto macroscopic mesh.

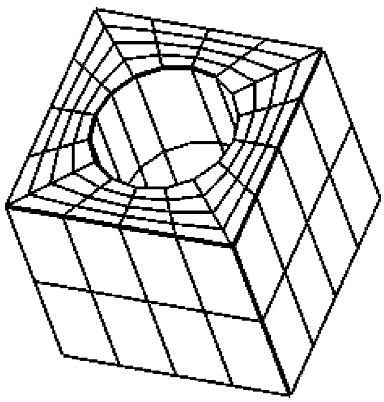

Fig. 11. Unit cell model for homogenization.

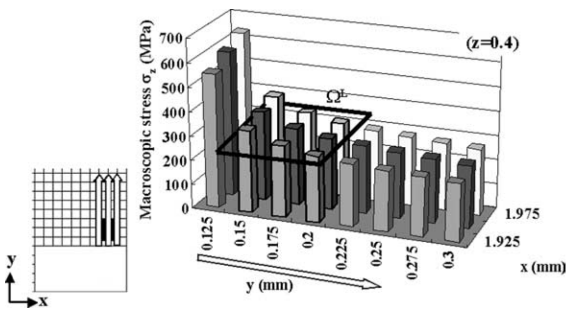

Fig. 12. Macroscopic stress near interface crack and microscopic region to be analyzed.

numerical error around Γ^{GL} does not lead to a critical problem in analyzing real materials with random microstructure.

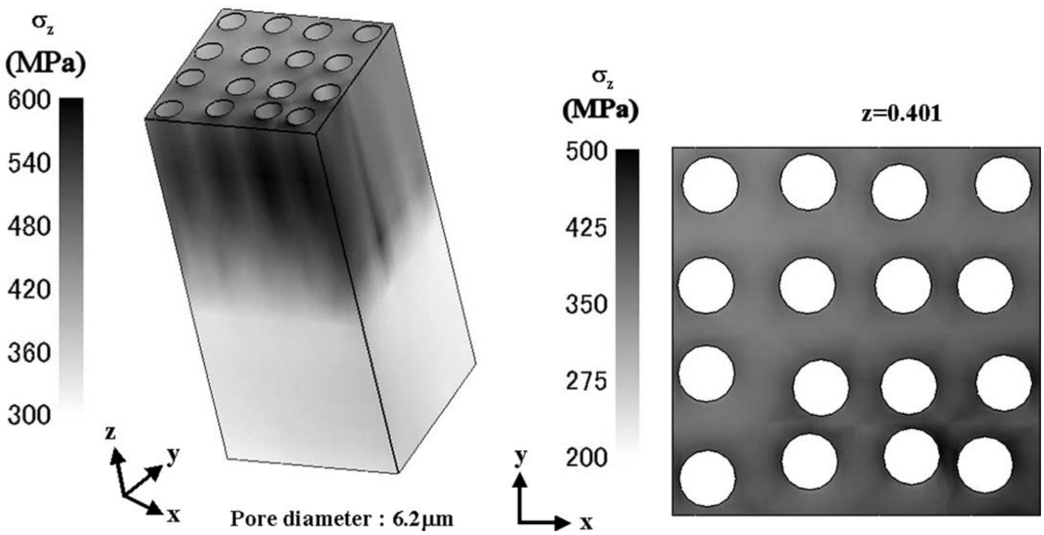

Fig. 13. Analyzed microscopic stress distribution by proposed three-scale method.

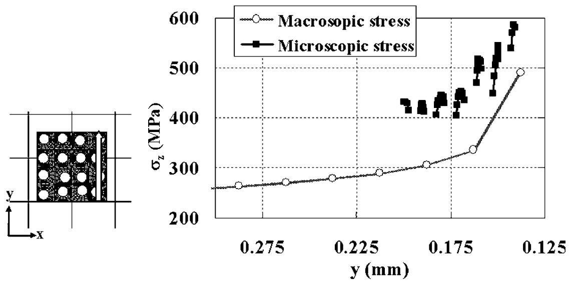

Fig. 14. Comparison of microscopic stress and macroscopic stress at crack tip.

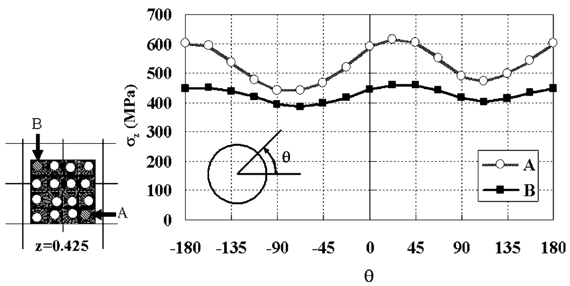

Fig. 15. Comparison of microscopic stresses in microscopic region.

It is interesting to note that the microscopic stress is non-periodic with respect to the microstructure model. This is advantageous compared to the conventional homogenization method. This is clearly indicated by the plot of microscopic stress shown in Fig. 14. The complex microscopic stress distribution is obtained because of the high gradient of macroscopic stress at the crack tip and also due to the pores. The

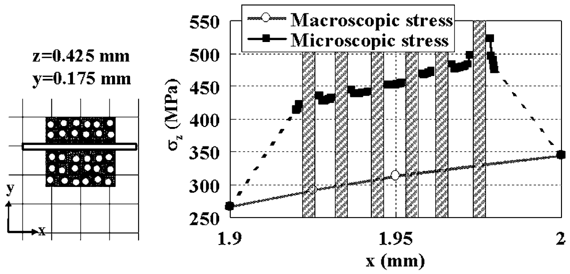

Fig. 16. Analyzed stress field in and around microscopic region showing discontinuity at boundary Γ^{GL}.

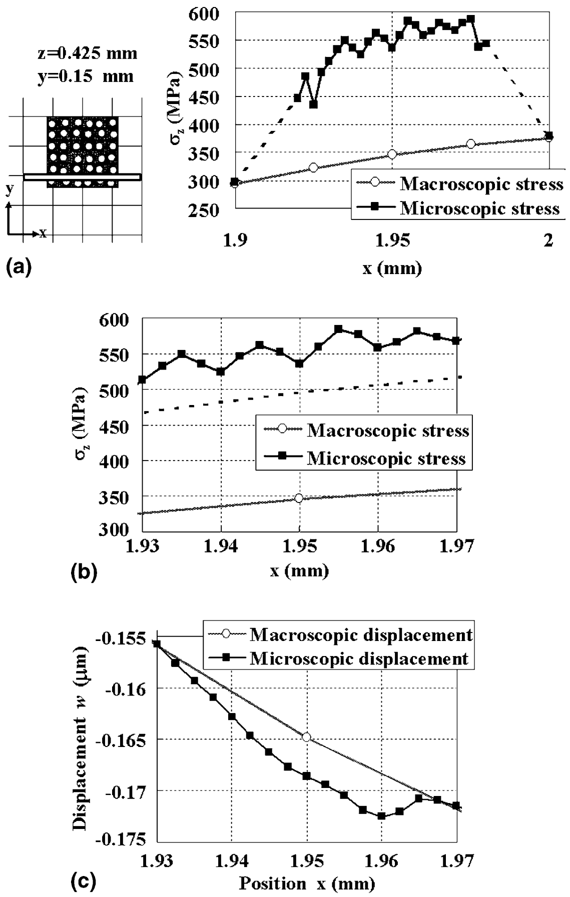

Fig. 17. Detailed distribution of analyzed stress and displacement near crack tip. (a) Comparison of macroscopic and microscopic stress. (b) Inner region of microscopic mesh. (c) Comparison of macroscopic displacements.

random dispersion of pores also influences the microscopic stress distribution. Fig. 15 shows the stress distribution around specific pores. The high macroscopic stress and the narrow gap between the neighboring pores contributed to the increase in microscopic stress.

Fig. 16 shows an example of the analyzed stress field by superimposing the microscopic mesh. The macroscopic stress, without using the mesh superposition method, has also been plotted. Due to the discontinuity of material models in the proposed method, the stress is not continuous at boundary Γ^{GL} and includes a numerical error. However, the boundary region to be excluded in stress evaluation is not very wide and the stress distribution in Fig. 13 is reliable. Another example is shown in Fig. 17. With respect to the inner region in Fig. 17(b), the microscopic stress is higher than the macroscopic stress by 1/(1 − porosity ratio) = 1/0.7 (dashed line). This is due to the randomness of pores. The macroscopic stress is the averaged one over much wider region. On the other hand, the present method provides more precise distribution in a microscopic region. By taking various dimensions of the microscopic region, the stress can be analyzed at arbitrary resolution microscopically. The consistency of the macro- and microscopic stresses are assured in this case, however it depends generally on the scale gap between the macro- and microscopic models and the limitations of the asymptotic homogenization. Moreover, the displacement field is also very complex as shown in Fig. 17(c). The periodicity of the stress field is lost in this local region due to the random dispersion of pores and the high gradient of macroscopic strain. By taking arbitrary microscopic region, the precise microscopic stress and displacement can be analyzed, which are deviated from the macroscopic ones near the fracture origin. These results indicate the necessity and importance of the microscopic stress analysis.

5. Conclusion

This paper described the synergetic application of the asymptotic homogenization and the mesh superposition methods to a three-scale 3D problem with scale mixing issue for various advanced materials. The heterogeneous microstructure, macroscopic component, and interface crack, whose representative dimension is between that of the microstructure and the component, were studied simultaneously. Differently from the conventional hierarchical modeling strategy, the finite element mesh superposition method was used to consider the interface crack, the microscopic heterogeneity, and the influence of the macroscopic boundary conditions. The use of the homogenization is essential to predict the consistent constitutive model accurately for complex 3D microstructure architecture together with the mesh superposition method. The microscopic stress can be analyzed under non-uniform macroscopic stress field with high gradient. The effect of the randomness of the microstructure was also considered, and it was found to influence the microscopic stress. To solve 3D problems by the mesh superposition method, a renumbering technique and out-of-core skyline method were employed. A numerical example with approximately 80,000 elements was discussed in this paper. The proposed three-scale finite element method enables us to analyze the microscopic behavior in locally and non-periodically heterogeneous region with arbitrary dimensions including crack, void, inclusion, etc. for various advanced materials and components.

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References

Benallal, A., Tvergaad, V., 1995. Nonlocal continuum effects on bifurcation in the plane strain tension-compression test. J. Mech. Phys. Solids 43, 741–770.

Buryachenko, V.A., Pagano, N.J., Kim, R.Y., Spowart, J.E., 2003. Quantitative description and numerical simulation of random microstructures of composites and their effective elastic moduli. Int. J. Solids Struct. 40, 47–72.

Caiazzo, A.A., Costanzo, F.C., 2001. Modeling the constitutive behavior of layered composites with evolving cracks. Int. J. Solids Struct. 38, 3469–3485.

Fish, J., 1992. The s-version of the finite element method. Comput. Struct. 43, 539–547.

Fish, J., Wagiman, A., 1993. Multiscale finite element method for a locally nonperiodic heterogeneous medium. Comput. Mech. 12, 164–180.

Fish, J., Yu, Q., 2002. Computational mechanics of fatigue and life predictions for composite materials and structures. Comput. Meth. Appl. Mech. Eng. 191, 4827–4849.

Fish, J., Shek, K., Pandheeradi, M., Shephard, M.S., 1997. Computational plasticity for composite structures based on mathematical homogenization: theory and practice. Comput. Meth. Appl. Mech. Eng. 148, 53–73.

Ghosh, S., Lee, K., Moorthy, S., 1996. Two scale analysis of heterogeneous elastic–plastic materials with asymptotic homogenization and Voronoi cell finite element model. Comput. Meth. Appl. Mech. Eng. 132, 63–116.

Ghosh, S., Lee, K., Raghavan, P., 2001. A multi-level computational model for multi-scale damage analysis in composite and porous materials. Int. J. Solids Struct. 38, 2335–2385.

Guedes, J.M., Kikuchi, N., 1990. Preprocessing and postprocessing for materials based on the homogenization method with adaptive finite element method. Comput. Meth. Appl. Mech. Eng. 83, 143–198.

Knockaert, R., Doghri, I., 1999. Nonlocal constitutive models with gradients of internal variables derived from a micro/macro homogenization procedure. Comput. Meth. Appl. Mech. Eng. 174, 121–136.

Ladeveze, P., 1995. A damage computational approach for composites: basic aspects and micromechanical relations. Comput. Mech. 17, 142–150.

Lee, K., Moorthy, S., Ghosh, S., 1999. Multiple scale computational model for damage in composite materials. Comput. Meth. Appl. Mech. Eng. 172, 175–201.

Lions, J.L., 1981. Some Methods in the Mathematical Analysis of Systems and Their Control. Science Press, Beijing.

Moulinec, H., Suquet, P., 1998. A numerical method for computing the overall response of nonlinear composites with complex microstructure. Comput. Meth. Appl. Mech. Eng. 157, 69–94.

Murata, K., Oguni, T., Karaki, Y., 1985. Supercomputer. Maruzen, Tokyo (in Japanese).

Nakasumi, S., Suzuki, K., Fujii, D., Ohtsubo, H., 2002. An elastic and elasto-plastic mixed analysis using overlaying mesh method. Trans. Jpn. Soc. Mech. Eng. 68, 603–610 (in Japanese).

Okada, H., Ninomiya, T., Sakasegawa, Y., Fukui, Y., Kumazawa, N., 2003. On mesoscale analysis for composite materials using s-FEM (some trials). In: Proc. Conf. Comput. Eng. Sci., Tokyo, vol. 8, no. 1, pp. 243–246 (in Japanese).

Rashid, M.M., 1998. The arbitrary local mesh replacement method: an alternative to remeshing for crack propagation analysis. Comput. Meth. Appl. Mech. Eng. 154, 133–150.

Robbins Jr., D.H., Reddy, J.N., 1996. An efficient computational model for the stress analysis of smart plate structures. Smart Mater. Struct. 5, 353–360.

Schraad, M.W., Triantafyllidis, N., 1997. Scale effects in media with periodic and nearly periodic microstructures, part 1: macroscopic properties. ASME J. Appl. Mech. 64, 751–761.

Shephard, M.S., Beall, M.W., Garimella, R., Wentorf, R., 1995. Automatic construction of 3-D models in multiple scale analysis. Comput. Mech. 17, 196–207.

Shinmura, D., Suzuki, K., Nakasumi, S., Fujii, D., Ohtsubo, H., 2002. A study on iteration method of global local analysis using overlaying mesh method. In: Proc. Conf. Comput. Eng. Sci., Tokyo, vol. 7(2), pp. 529–532 (in Japanese).

Takano, N., Uetsuji, Y., Kashiwagi, Y., Zako, M., 1999. Hierarchical modelling of textile composite materials and structures by the homogenization method. Model. Simul. Mater. Sci. Eng. 7, 207–231.

Takano, N., Ohnishi, Y., Zako, M., Nishiyabu, K., 2000a. The formulation of homogenization method applied to large deformation problem for composite materials. Int. J. Solids Struct. 37, 6517–6535.

Takano, N., Zako, M., Ishizono, M., 2000b. Multi-scale computational method for elastic bodies with global and local heterogeneity. J. Computer-Aided Mater. Design 7, 111–132.

Takano, N., Ohnishi, Y., Zako, M., Nishiyabu, K., 2001a. Microstructure-based deep-drawing simulation of knitted fabric reinforced thermoplastics by homogenization theory. Int. J. Solids Struct. 38, 6333–6356.

Takano, N., Zako, M., Okazaki, T., 2001b. Efficient modeling f microscopic heterogeneity and local crack in composite materials by finite element mesh superposition method. JSME Int. J. 44, 602–609.

Takano, N., Kimura, K., Zako, M., Kubo, F., 2002. Multi-scale analysis and microscopic stress evaluation for ceramics considering the random microstructures. Trans. Jpn. Soc. Mech. Eng. 68, 1046–1053 (in Japanese).

Takano, N., Zako, M., Kubo, F., Kimura, K., 2003a. Microstructure-based stress analysis and evaluation for porous ceramics by homogenization method with digital image-based modeling. Int. J. Solids Struct. 40, 1225–1242.

Takano, N., Zako, M., Okuno, Y., 2003b. Multi-scale finite element analysis for joint members of heterogeneous dissimilar materials with interface crack. J. Soc. Mater. Sci. Jpn. 52, 952–957 (in Japanese).

Terada, K., Kikuchi, N., 2001. A class of general algorithms for multi-scale analyses of heterogeneous media. Comput. Meth. Appl. Mech. Eng. 190, 5427–5464.

Torquato, S., 1998. Morphology and effective properties of disordered heterogeneous media. Int. J. Solids Struct. 35, 2385–2406.

Triantafyllidis, N., Bardenhagen, S., 1996. The influence of scale size on the stability of periodic solids and the role of associated higher order gradient continuum models. J. Mech. Phys. Solids 44, 1891–1928.