Transactions of the 15th International Conference on
Structural Mechanics in Reactor Technology (SMiRT-15)
Seoul, Korea, August 15-20, 1999

Coupled Multi-Level Modeling for Hot Deformation of Materials

Tatsuhiko Aizawa and Fujio Tsumori

University of Tokyo, Japan

ABSTRACT

Multi-level mechanical model is indispensable to describe the microstructure evolution of materials together with the macroscopic geometric change of product. In particular, coupling interaction between or among deformation, temperature and mass-diffusion transients is needed to deal with hot deformation and flow behavior of materials. In the present paper, theoretical fundamentals are introduced with some comments on the computer installation of this modeling to the parallel computer system. The sintering process simulations are performed to demonstrate the validity and effectiveness of the present approach.

INTRODUCTION

Materials processing design becomes an important tool to improve reliability and integrity of P/M parts and members. Various researches have been reported in the literature [1] not only for the powder compaction and forming analysis but also for the sintering analysis. In the former, both densification process and powder mobility/flow behavior are highlighted to quantitatively evaluate the experimental results. Both the granular/powder modeling [2] and the continuum mechanics modeling [3] are widely used; in the granular modeling, since each powder or its agglomerates are represented by an element, the effect of powder size distribution and morphology on the compaction behavior is directly simulated both in two and three dimensional situations. Using the constitutive equations where the powders are approximated by a porous continuum, the stress state and its change can be described together with densification by the rigid-plastic and elasto-plastic models. In the latter, the sintering analysis method is classified into three types: a) Continuum mechanics modeling [4], b) Granular/powder modeling [5] and c) Microscopic modeling [6]. The first two models were developed by the same concept as used in the powder compaction analysis. The points to be noticed are: [1] Rational constitutive model to describe the evolution of density during sintering must be a priori obtained by experiments, and, [2] Various diffusion and migration mechanism can be

taken into account, but no external stresses nor boundary conditions have any relations with that microscopic model. In actual situation, sufficient amount of experimental data cannot be prepared for sintering analysis for research, and, macroscopic sintering process conditions have significant influence on the time evolution of microstructure.

As a new approach to sintering analysis, the multi-level modeling [7] has been proposed and developed not only to investigate the effect of parameters on the sintering process but also to describe the microstructure evolution during sintering. Since the constitutive equation for matrix materials is only necessary, the fundamental data for each alloy or compound material is commonly utilized, so that no experimental data are needed once those data are cited. As illustrated in Fig. 1, the sintering behavior can be represented by the coupled hierarchical modeling; the effect of temperature history on the geometric shrinkage is directly considered through the coupling analysis. In the present paper, the fundamentals in the present coupled macro-micro modeling are first stated with comments on the homogenization theory and the unit cell. The uncoupled multi-level modeling for sintering of steel powder compacts is compared with the experimental measurement of densification in order to quantitatively demonstrate the validity of the present method. Through application of the coupled multi-level modeling, the effect of thermal gradient and externally applied pressure on the geometric configuration is discussed. With respect to the computational mechanics, natural adaptivity of this modeling to parallel computing is stressed in order that the complex problems appearing in the sintering behavior should be represented and solved by the multi-level modeling.

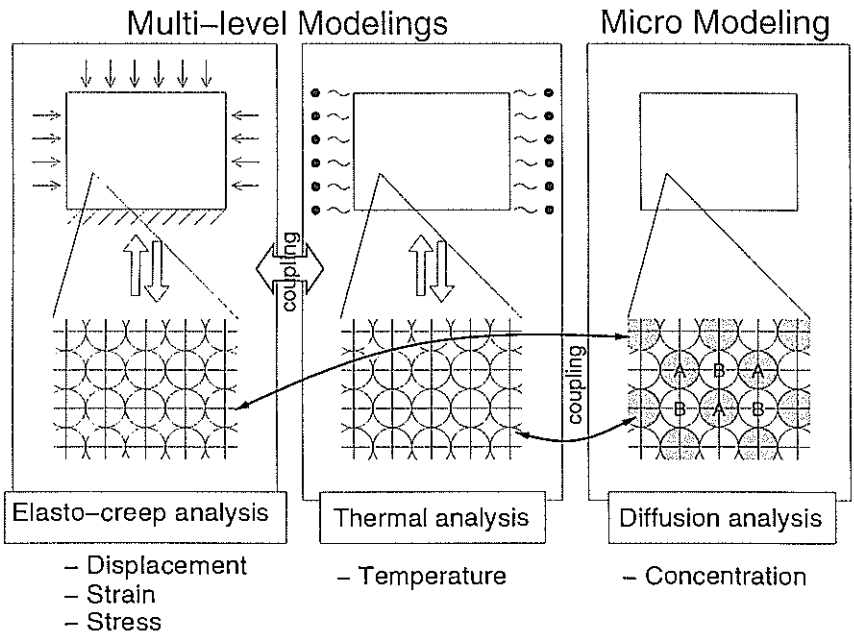


Figure 1: Coupled multi-level modeling for the sintering analysis.

COUPLED MULTI-LEVEL MODELING

Different from the conventional micromechanics, which stands on the random representative expression, a porous medium in sintering is assumed in this modeling to be an assembly of periodically structured materials with different periodicities. The points to be discriminated from usual micromechanical approximation by using the periodic structure are: 1) Any type of unit cells having its own unique periodicity should be allowed to represent local microstructure or porosity structure in materials, 2) Sintered material with complex structural evolution in its inside can be modeled into a coupled. multi-level representation, each of which can be formulated by using different unit cells and periodicities. In the present paper, the homogenization method is used as a main theoretical principle to construct the multi-level modeling. As illustrated in Fig. 2, the targeting material to be sintered is represented by an assembly of finite elements at the top level of this multi-level modeling, where the unit cell corresponds to a periodic structure in the lower level. If this second level still had a certain periodic structure, further lower level modeling could be made. Until no physical meaning can be found for the inter-level connection between successive two models, this downward hierarchical structuring could continue recursively. The mechanical consistency in this multi-level modeling requires for the upward validation of the physical quantities and properties: 1) Physical quantities at the base-level model are uniquely defined by direct solution of the goveming equation, and the constitutive relations in the solid mechanics are used as proper properties, and, 2) Physical quantities and properties at the higher level are estimated by averaging on the basis of the lower-level structure. Hence, various physical models can be selected to describe the fundamental processes in sintering.

Two level modeling is employed here to describe the sintering behavior: 1) Macro model to represent the geometric change of a bulk material in sintering, and, 2) Micro model to predict the local shrinkage of microstructure. To be noticed, various physical phenomena influence on the sintering: deformation of materials at the elevated temperature, temperature distribution and heat flux gradients, diffusion mechanism, and so forth, as before-mentioned in Fig. 1. The variational equation and inequlity methods in the applied mechanics enable us to create a theoretical frame to represent the above macro-micro modeling by the hierarchical relation of variational equations and the coupling between variational equations and inequilities. The variational equations in the visco-elastic or elasto-creep model for deformation of materials and those in thermal conduction for heat transfer are respectively used in formulation, so that the above hierarchical and coupled model is represented by the relation of variational equations in Fig. 3. The variational equations in the micro model is nearly equal in formal to the conventional formulation except for the prescription of the periodic boundary conditions. On the other hand, the homogenized stiffness and conduction coefficient tensors and creep stress tensor are used in the macro model to calculate the average displacements, strains, stresses and temperature. These averaged physical quantities are transferred to the micro model to update the physical quantities by adding the local perturbed contribution in the micro model to the above averaged values.

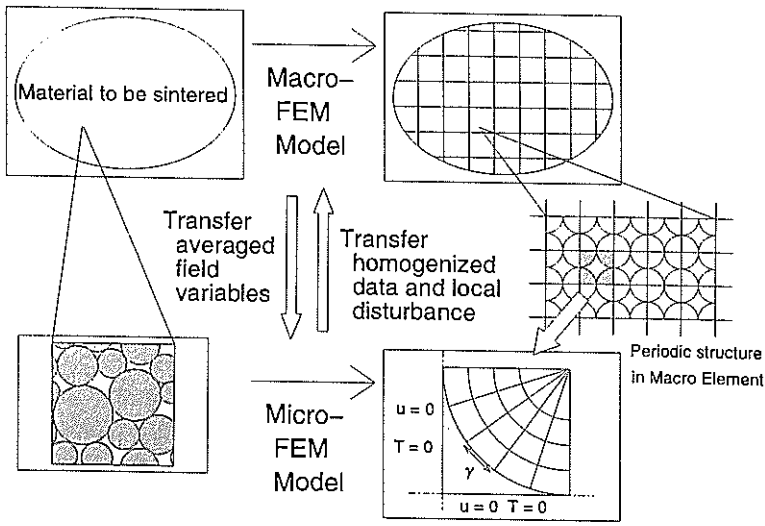
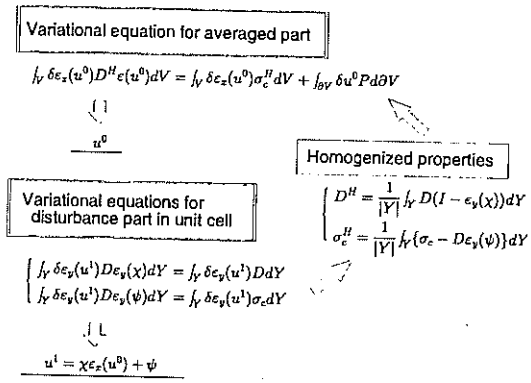


Figure 2: Macro model and micro model (unit cell model) for the sintering analysis.

(a)



(b)

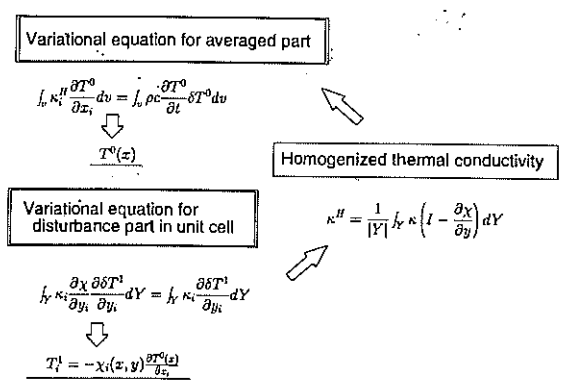


Figure 3: Hierarchical structre for the macro-micro analysis: (a) Visco-elastic deformation system, and, (b) Heat transfer system.

MULTI-LEVEL SIMULATION SYSTEM

The present multi-level simulation system was constructed by using C++ language, which is one of the object oriented programming language. Under the accommodation software for the parallel computing, the above system can work on the several to hundreds of engineering work stations. The essential part of this system lies in the class MLM (Macro-Linkage-Micro) between two successive models. The related data are controlled in the unit of this class: e.g. "Class-Node" denotes for the data block relating the node data, and, "Class-Element" the element data block. Various data types are allowed in each-class datum: scalar, vector and matrix. The arithmatic operations for inner product or multiplication are also defined as the class-operation. Then, little labors are necessary for extension of the two dimensional analysis to the three dimensional analysis; the class-data structure has nothing to do with the dimesional change. In addition, once the class-data structure is built in the system for two-structured model or only macro-micro modeling, any hierarchically structured model can be deal with by using the common class- data structure.

For the parallel computing on the group of engineering work stations (EWS), this multi-level modeling can work by simple broadcasting and data collection routine. As depicted in Fig. 4, the common data are distributed to each EWS, which is in charge for one micro model. Since no data interactions take place among these micro models, the calculation for each micro model advances independently. The analyzed micro model data are collected and transferred to the macro model. In the macro model, the calculation must be also done independently from the micro models; the averaged physical quantities obtained by this calculation are to be broadcast to each EWS.

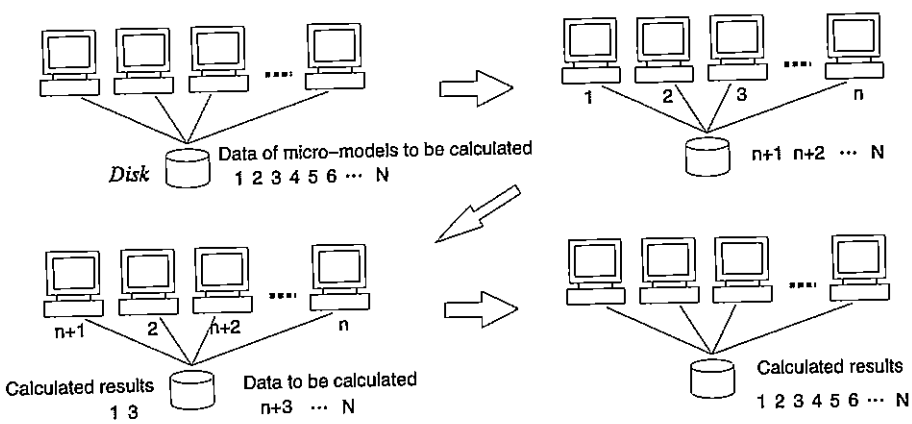


Figure 4: Schematic view for parallel computing in the multi-level modeling.

SINTERING ANALYSIS OF POROUS MEDIA

In practice, both the temperature and pressure conditions have significant influence on the geometric deformation and microstructure evolution. In the coupled multi-level modeling, additive physical properties such as the thermal conductivity and specific heat are only necessary to the fundamental data for uncoupled model, where the elastic moduli and the constitutive equation for creep of matrix materials are only necessary for sintering analysis. The process conditions are considered as the initial or the boundary conditions: the applied stress pressure is considered in the macro model as the mechanical tractions on the prescribed surface of materials, and, the temperature and heat flux are prescribed by the initial and boundary conditions. On the other hand, the surface tension in sintering is taken into account in the micro model by the boundary condition.

Two typical sintering processes were employed for a numerical example to understand the effect of externally applied pressure on the geometric change during sintering. Figure 5 summarizes the initial configuration of materials to be sintered. The porous material is sintered at the presence of thermal gradient without and with the external pressure. To be commonly noted in the above models, the initial diameter of pore is 20 μm, and, porosity distributes regularly in materials. Figure 6 depicted the geometric change of materials in sintering with the variation of stress state for two models. In the free sintering when no pressure is applied and temperature distribution is uniform, since homogeneous shrinkage takes place even in local, little or no bending is observed in geometry. Due to the thermal gradient in materials, the porous medium was forced to be bent upward since the local shrinkage advances at the higher temperature side. On the other hand, when the pressure was externally applied, no bending was observed; this is because the external stress becomes more dominant to sintering than the surface tension in local.

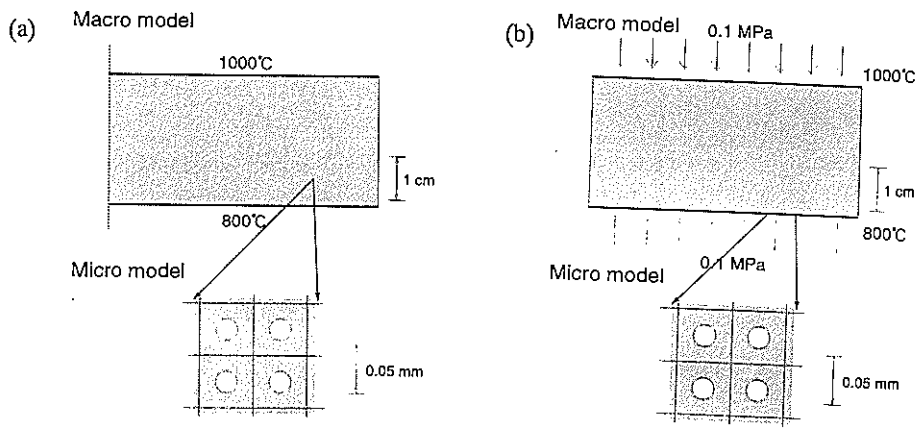


Figure 5: Two models to investigate the effect of process conditions on the geometric change of a material during sintering: (a) without any externally applied pressure, and, (b) with the applied constant pressure by 0. 1 MPa.

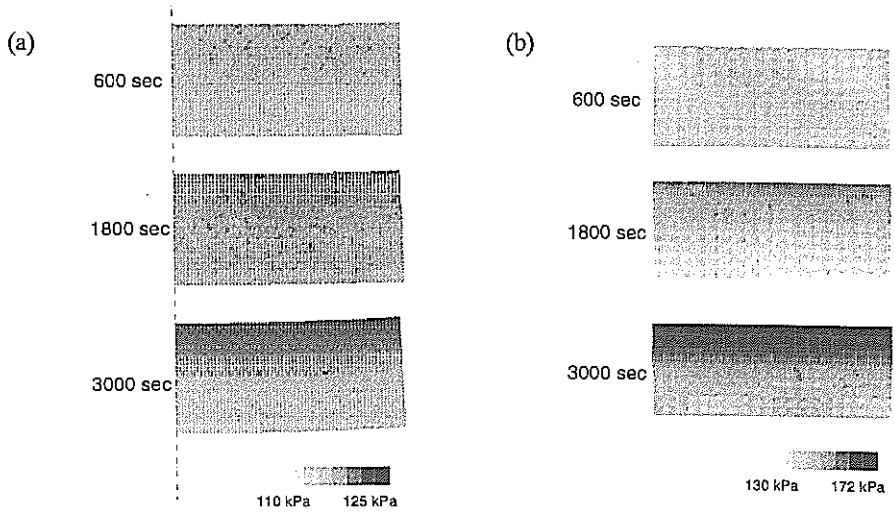


Figure 6: Geometric configuration of product with the evolution of stress state during sintering: (a) without any externally applied pressure, and, (b) with the applied constant pressure by 0. 1 MPa.

COUPLING BEHAVIOR IN HOT DEFORMATION OF MATERIALS

The hipping (hot isostatic pressing or HIP) process has been frequently utilized for fully densification of various porous materials and powder compacts. For verification test of the present macro-micro modeling to trace the densification or shrinkage process, this hipping process simulation is employed as an example. Figure 7 shows the benchmark test conditions where the austenitic stainless steel 316 L powder compact is hipped. Table 1 summarizes the necessary computational conditions; the thermal dependency of elastic constants and the constitutive equations experimentally obtained for solid SUS 316 L specimens were directly used as input data. The point to be noted here is that no materials properties nor constitutive equations for the porous media or the powder compact should be necessary for the present analysis. As before mentioned, the conventional continuum mechanics modeling requires for those data in quantitative simulation.

Although the deformed shape can be also predicted by the present method, just like the conventional methods, only the time history of volumetric shrinkage rate is compared with the experimentally measured results by the dilatometer. As shown in Fig. 8, both time histories are in fairly good agreement with each other up to the time when most of preform is nearly-fully densified in hipping. In actual experiments, the residual porosities gradually disappear themselves, and approaches to zero. Corresponding to this densification, the stroke reduced itslef monotonically and turned back by unloading. While, in simulation, complete reduction of cavities into zero volume cannot be attained by the finite element model in the Lagrangian frame. Here, even after t = 1. 3 ks in Fig. 8, the volume shrinkage rate abruptly decreases in experiments, while the calculated rate monotonically increases with time.

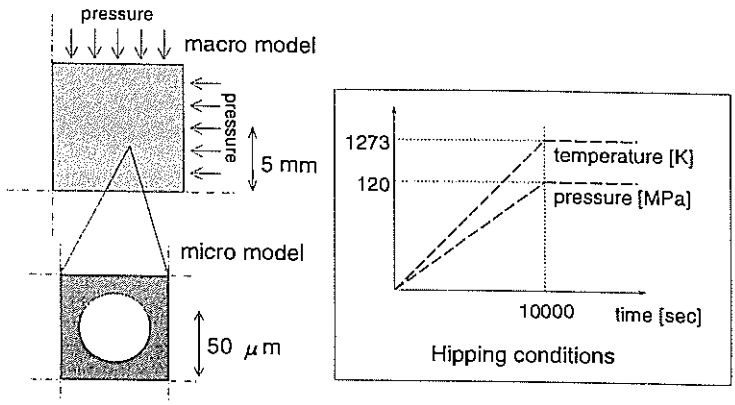


Figure 7: Benchmark test of hipping process simulation.

Table 1: Computational conditions of hipping process for the austenitic stainless steel 316 L powder compact.

Young's modulous	
$194000 - 81.4T$ (T<700 ℃)	MPa
Poisson's ratio	
0.3	
Thermal conductivity	
$13.651 + 0.01434T$	W/mK
Specific heat	
$465.45+0.21045T+8.6641\times10^{-7}T^2$	J/kgK

(Above 700 ℃, Young's modulus is supoosed to decrease linearly to zero at melting temperature 1375 ℃.)

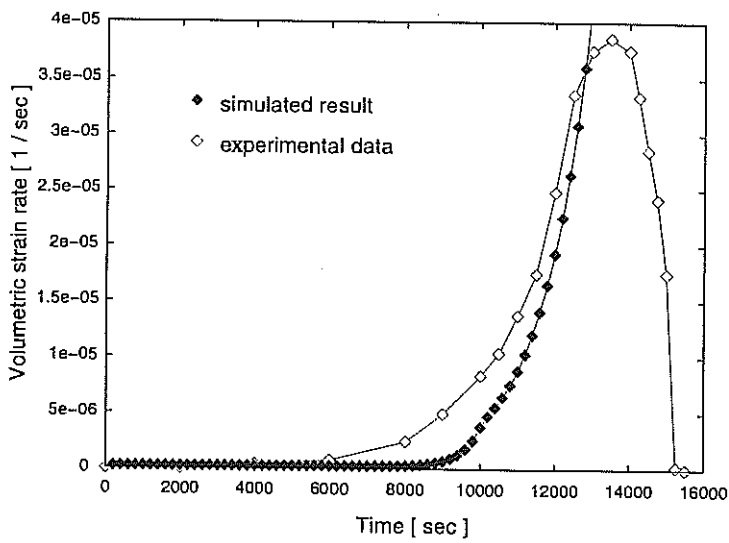


Figure 8: Comparison of shrinkage history in hipping between the calculated and experimental results.

DISCUSSION

One of the most attractive features for the present multi-level modeling lies in the theoretical prediction of stiffness and strength for the porous medium or the powder compact in sintering. In case when the elasto-creep modeling is used for deformation analysis of sintering, the elastic moduli of the sintered powder compact can be estimated in the function of the porosity. Figure 9 compared the calculated Young's and shear moduli from the homogenized stiffness matrix and the experimentally measured elastic moduli by using the ultrasoic measurement. Both are in fairly good agreement with each other. The simulated shear modulus became a little lower than the experimental results. This might be because the unit cell with the regularly distributed perforate was employed in computation to represent the more complicated microstructure in the actual sintered product.

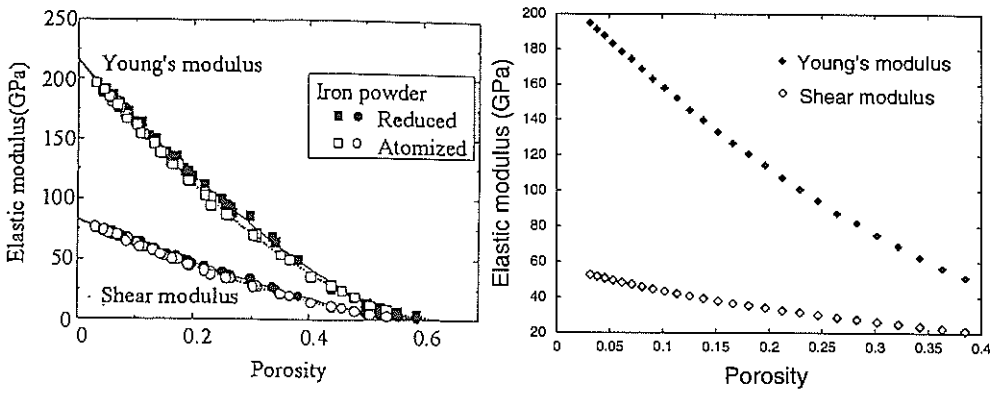


Figure 9 Comparison of the elastic moduli between the calculated results by the present method and the experimentally measured data.

When using the regularly shaped unit cell is used to represent the microstructure, the calculated results are equal to the analytically estimated results by using the micromechanics in elasticity. For an example, both estimated stiffness tensors are just in agreement for the regularly perforated elastic body. Even for those regular microstructure, nonlinear stiffness can be only predicted by the present method. Hence, the conventional micromechanics can be replaced by the multi-level modeling with sufficient knowledge in selecting the unit cell and in nonlinear formulation. In the present study, only visco-elastic or elasto-creep models were utilized as the constitutive model to deal with hot deformation. Since any type of functional representations can be available for equations, the present approach is to be directly applied to various structural analyses at the elevated temperature. Besides the viscoelasticity, many kinds of mechanical models are useful in the same formulation by the initial strain method. Furthermore, although the updated Lagrangian frame was used as the coordinate system, the Eulerian frame is recommended to use in dealing with the fracture, decomposition, cavitation problems by the multi-level modeling.

CONCLUSION

The materials design of porous media and cellular matters requires for a new method to create the theoretical bridge between the microstructure in those materials and their mechanical functionality. The present multi-level modeling provides us the first step toward the promising bridge to understand the relation between microscopic structure and macroscopic functionality. As discussed before, rational selection of a unit cell is very important when applying the present method to actual problems. Since the adaptive unit cell to microstructure in reality is hidden in materials, the other experimental measurement should be necessary at least to determine the length of periodicity. Author insisted the acoustic homogenization method [8] to rationally estimate the periodicity of hidden unit cell. A series of studies [9] are still needed to biuld up how to generate the adequate unit cell. In general, the multi-dimensional analysis requires for super-large computation where the time evolution of physical quantities and properties must be traced with hundred thousands of degrees of freedom in total. Hence, parallel computing is indispensable; the promising algorithm for multi-dimensional analysis should have a parallel computing context in itself. The multi-level modeling is thought to be suitable to nonlinear multi-phase or multi-material problems which need large computation.

REFERENCES

1) S. Tamura: Powder flow, consolidation and sintering analysis in the powder metallurgy. PhD Thesis, University of Tokyo (1995).
2) T. Iwai: Development of granular modeling for powder injection molding design and analysis. PhD Thesis, University of Tokyo (1997).
3) J. Terziyski: Three dimensional . PhD Thesis, University of Tokyo (1994).
4) J.I. Martinez-Herrera and J.J. Derby: Analysis of capillary driven viscous flows during the sintering of ceramic powders. AIChe Journal. 40 (1994) 1794-1802.
5) F. Tsumori, T. Aizawa and J. Kihara: Sintering analysis by the granular modeling. J. Jpn Powder and Powder Metallurgy. 42 (1995) 501-509.
6) V. Tikare and J.D. Cawley: Numerical simulation of grain size distribution in liquid phase sintered materials. Ceramic Transaction 69 (1997) 187-194.
7) F. Tsumori: Multi-level modeling for sintering analysis with consideration of inner mechanism. PhD Thesis, University of Tokyo (1999).
8) T. Aizawa: Superplastic forging analysis by the multi-level modeling. Materials Science Forum. 304-306 (1999) 621-630.
9) T. Aizawa: Macro-micro modeling to describe the porous agglomerated ore. ISIJ (1999) (to be submitted).