复合材料随机多尺度分析数值方法与工程应用

Stochastic Multiscale Simulation Method and Application for Composite Material

文 聘 ◎著

中国铁道出版社
CHINA RAILWAY PUBLISHING HOUSE

复合材料随机多尺度分析数值方法与工程应用

Stochastic Multiscale Simulation Method and Application for Composite Material

文聘 著

中国铁道出版社
CHINA RAILWAY PUBLISHING HOUSE

内 容 简 介

本书全面系统地论述了材料性能多尺度分析方法与摄动展开渐进均匀化方法的基本理论，建立了以概率随机数值方法为基础的等效弹性力学性能分析方法实现过程，较为全面地实现了对材料二维、三维弹性应力场的随机模拟。另外，本书还探讨了多孔材料、多相复合材料随机等效弹性力学性能统计分布特征，并提出了其相应的模型。

本书适合作为普通高等学校力学专业或土木工程专业的教材，也可作为材料性能多尺度分析方法的参考书，还可供相关专业技术人员参考。

图书在版编目(CIP)数据

复合材料随机多尺度分析数值方法与工程应用＝Stochastic Multiscale Simulation Method and Application for Composite Material:英文/文聘著. —北京:中国铁道出版社,2019.1

ISBN 978-7-113-24326-5

Ⅰ.①复… Ⅱ.①文… Ⅲ.①工程材料-结构性能-分析方法-英文 Ⅳ.①TB303

中国版本图书馆 CIP 数据核字(2018)第 280541 号

书　　名：复合材料随机多尺度分析数值方法与工程应用
Stochastic Multiscale Simulation Method and Application for Composite Material
作　　者：文聘　著

策　　划：曾露平　　读者热线：(010) 63550836
责任编辑：曾露平
封面设计：刘　颖
责任校对：张玉华
责任印制：郭向伟

出版发行：中国铁道出版社（100054，北京市西城区右安门西街 8 号）
网　　址：http://www.tdpress.com/51eds/
印　　刷：北京盛通印刷股份有限公司
版　　次：2019 年 1 月第 1 版　　2019 年 1 月第 1 次印刷
开　　本：787 mm×1 092 mm　1/16　印张：9　字数：224 千
书　　号：ISBN 978-7-113-24326-5
定　　价：48.00 元

版权所有　侵权必究

凡购买铁道版图书，如有印制质量问题，请与本社教材图书营销部联系调换。电话：(010) 63550836

打击盗版举报电话：(010) 51873659

此为试读，需要完整PDF请访问：www.ertongbook.com

Preface

This book aims at introducing a probabilistic multiscale simulation based approach for design and fabrication of materials considering microstructural uncertainties. It is apparently clear from the extant literature that the parameters to capture microstructural uncertainties are unclear, and it is therefore very challenging to frame the research problem either using the homogenization process or using a statistical model.

Accordingly, a novel first-order perturbation based stochastic homogenization (FPSH) method is developed to incorporate material properties uncertainties in three-phase constituents by setting random parameters in probabilistic distribution. When newly considering non-parametric geometrical fluctuation and/or other miscellaneous errors, the distribution derived above for macroscopic property is calibrated and re-written in the mixture distribution. The probabilistic computational approach leads to the decrease in dimension of uncertain parameters in the sampling space.

In the model, mainly, two types of uncertain parameters are described mathematically to simulate the fluctuation of microstructural geometry i. e. one is the parametric uncertainties used in FE model that are measurable; the other one is the non-parametric uncertainties used in FE model, which are completely random and can't be measured.

The fabricated prototype was compared with the simulated predictions which reveals some differences. Consequently, the fabricated microstructure was fed back to the simulation model. It was discovered that the experimental data can be used to predict the fabricated morphology of microstructure.

As a testbed study, a coated particulate material was modelled as a demonstrative example of above simulation method for three-phase material. The design option was drawn for particle radius and coating thickness in the case of 5%, 50%, 95% probabilistic response surface through probability distribution. Moreover, based on probabilistic response surface, the probabilistic sensitivity was provided a robust design if we choose to have smaller particle radius and coating thickness will result in non-sensitive design to the uncertainties in materials properties and geometrical fluctuation at microscale.

To simplify the problem, a spherical porous material was modelled. It was noticed that significant difference maybe anticipated in obtaining macroscopic elastic property even if the porosity ratio is similar to what's predicted by stochastic method and conventional methods, which is where the proposed method provides superior predictions.

Furthermore, the application in selective laser sintered lattice structure is shown to obtain the deviation of apparent compressive stiffness when considering the variation of manufacturing conditions and constituent material.

It was concluded that the proposed simulation framework can be used generally for studying a range of engineering problems related to fabrication of real world materials to improve the design and fabrication parameters in order to improve the product's reliability.

This book was written by Pin Wen from Wuhan University of Technology, censored by professor Naoki Takano from keio university. It was funded by China Postdoc Science Fund(2017M620550) and Chaoyang District of Beijing Postdoc Science Fund.

I would like to thank my postdoctoral supervisor Professor Qingsheng Yang and Hongling Ye for providing me an opportunity and enabling me to write what I research. The work in chapter 4 and chapter 5 has received help from graduate students from Keio University and I would like to show my great appreciation to Daichi Kurita and Senichiro Yokota and Akimoto Shusuki. I thank my husband Mr Zuling Liang for proofreading the draft.

Due to the shortage of time, there may be some mistakes in the book. I greatly thanks readers to send email to me and improve the quality of book.

Author

January 2018

Contents

Chapter 1 Overview

1.1 Motivation

Heat insulating material has been calling high attention in the automobile engine to prevent the energy loss and increasing the fuel usage. With the development of new material design, this project has arisen to propose a new microstructure design to improve the macroscopic properties of heat insulating capacity. One of the challenge is the multifunctional target of this new material. Because the material should bear high pressure and at the same time high temperature in the inner chamber. At this double high requirement, it appears no design solution as shown in Fig. 1. 1. 1. It need to raise up the properties by designing and controlling microstructure in a better way. Thus the new microstructure can raise up both mechanical and thermal properties when some certain porosity ratio can be controlled after a specific processing in Fig. 1. 1. 2. The prototype of this new material has been made in one motor company. However there is a big gap between numerically designed material and manufactured one. When evaluation of the prototype was discussed to determine if it is appropriate to run a product line to fabricate this material reliably, the decision was stopped due to the high risk.

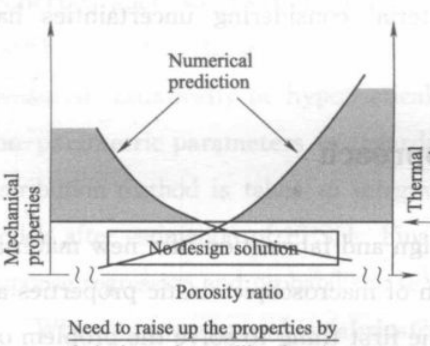

Fig. 1. 1. 1 Relationship between mechanical and thermal properties and porosity ratio

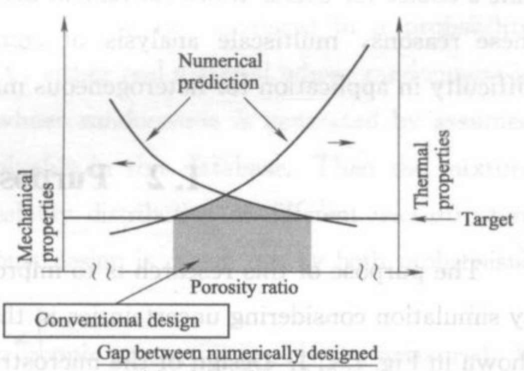

Fig. 1. 1. 2 Feasible solution space after improvement of microstructure design

The reliability design strategy is impelled to improve the conventional design. Uncertainties modeling is considered when multiscale method is used to predict the lower and upper bounds for new material design in Fig. 1. 1. 3. Although, homogenization, as a multiscale method has been reported to be effective and validated in prediction of proper randomness in the microstructure by previous researchers, not much research has been reported for homogenization incorporating uncertainties in modeling at microscale.

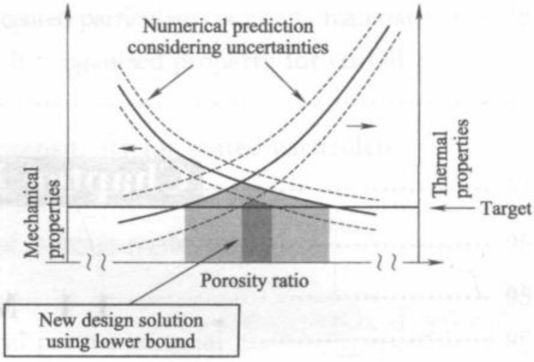

Fig. 1. 1. 3 New design solution considering uncertainties at microscale

Although Monte Carlo methods are widely used, it becomes impractical for computationally expensive models because it requires a large number of samples, and each sample requires expensive computational model. Repeating thousands of finite element models using input values generated by sampling strategy is far beyond current computational sources when more comprehensive multiscale model is considered. Although there are many approximation methods to reduce the computational cost, all of them introduce some kinds of optimal strategy of sampling points, such as Markov Chain Monte Carlo methods. Therefore, it would be desirable to propose a new method to combine stochastic theory and multiscale method to simulate material properties.

The complexity in uncertainties modeling for microstructure of composite material prevents not only the homogenization process, but also the statistical study because the parameters to describe the uncertainties of microstructures are not clear. In addition, the feasible solution space is filled by probability design points. That will make it difficult to take a choice for users. More convenient design choice should be made for users. Because of these reasons, multiscale analysis of composite material considering uncertainties has difficulty in application for heterogeneous materials.

1. 2 Purpose and approach

The purpose of this research is to improve the design and fabrication of a new material by simulation considering uncertainties in the prediction of macroscopic elastic properties as shown in Fig. 1. 2. 1. Design of the microstructure is the first thing to solve the problem on how the geometrical parameter and constituent materials and so on should be selected. To use the developed design methodology, the microarchitecture or morphology must be given. In this study, it is assumed that an expert engineer has already set a target microstructure with arrangement of inclusions based on his past experience and knowledge. Another choice is to use a topology optimization technique. Therefore, to give the morphology first is not a serious limitation. The design problem is defined that the macroscopic Young's modulus and shear modulus exceed the given required values.

If only topology of the microstructure is given, then the geometry can be a design parameter. The constituent material is another design parameter using its Young's modulus and shear modulus at the microscale. In some cases when the constituent material is selected, the variability in the geometry such as particle radius is supplied. In that case, the level of variability can also be included in the design parameters in the proposed method. This is practical and very useful. Therefore, the bottom block in Fig. 1. 2. 1 play an important role to connect the design and properties of a new material.

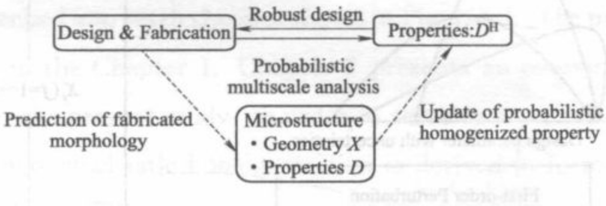

Fig. 1. 2. 1 Purpose for design and fabrication of a new material

In order to correlate the microstructure with macro properties in the right corner in Fig. 1. 2. 1, the first objective of this research is to develop a probabilistic homogenization methodology to incorporate the random parameters $\alpha_1, \alpha_2, \alpha_3$ in physical properties $[\boldsymbol{D}]$ at microscale for three-phase composite material. The random parameters to describe the constituent material properties at microscale are assumed in a probability density function. The first-order perturbation based stochastic homogenization (FPSH) method is proposed. Effective elastic properties such as macroscopic Young's modulus are to be calculated in a probability distribution. For the geometrical fluctuation in X, either real material whose randomness is measured statistically or hypothetical material whose randomness is generated by assumed non-parametric parameters is regarded to be solvable in this database. Then the mixture distribution method is taken to integrate the probability distribution of different microstructure models after estimation of FPSH. Finally, the robust design is drawn out by both probabilistic response regression and probabilistic sensitivity analysis.

When a new material is fabricated, the macroscopic properties are always measured. If the prediction agrees with measurement (yes in Fig. 1. 2. 2), the proposed method is perfectly confirmed. However, since uncertainty setting needs priori estimation of unknown factors, if the obtained properties are less than regressed values (no in Fig. 1. 2. 2), an update algorithm was proposed, which implies the fabricated microstructure. The merit is that no costly observation of microstructures is needed.

此为试读,需要完整PDF请访问: www.ertongbook.com

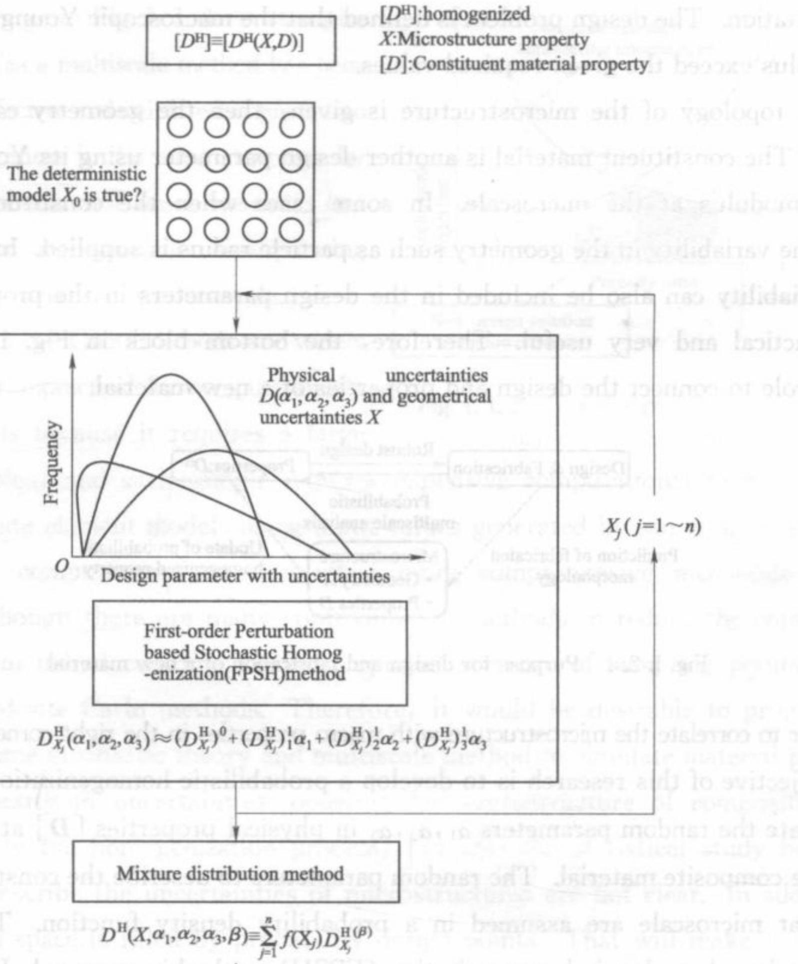

Fig. 1. 2. 2 Procedure of proposed approach

Furthermore, the difference between the developed design method and the conventional deterministic one lies in the much less failure probability. If 95% reliability curve (surface) is used, the proposed strategy can assure the high probability of success within few experimental trials and can save the cost away from a tons of testing trails. Moreover the sensitivity analysis can provide an insensitive domain of design variables that can change the parameters less sensitive to manufacturing variation.

1.3 Organization of thesis

This thesis is organized into seven chapters shown in Fig. 1.3.1. The motivation, purpose and approach are written in the Chapter 1. Chapter 2 presents an overview of the background information related to the present study, in order to serve as a prelude to the topics covered in later chapters. A new stochastic homogenization is derived in formulas from conventional two-scale homogenization. The theory incorporates parametric uncertainties in constituent material properties at microscale and propagates into macroscopic properties in a probability distribution. In Chapter 3, when the geometrical fluctuation is considered to be incorporated into the probabilistic homogenization, the mixture distribution and calibration is derived. The Monte Carlo method is widely used for uncertainty modeling of fluctuated microstructure geometry. Different from Monte Carlo method, probabilistic homogenization method proposed here has reduced the dimensions of uncertainties and make it possible to consider both analog (continuous) and digital (discrete) uncertain parameters. Chapter 4 explains computational material design methods for microstructure design and fabrication of heterogeneous material. The parameterization modeling in that chapter is used to identify geometrical uncertainties. A fabrication prototype is made and measured in a virtual experimental way. A comparison between the predicted results and measured result is also discussed. The update of prediction by experimental data is proposed then and validated to make the prediction closer to measured result. Finally there are two demonstrative numerical examples in Chapter 5 and Chapter 6. It is believed that the result of probabilistic response regression and probabilistic sensitivity provide a guidance for new material manufacturers. Findings, limitations, and future works related to the present study are described in Chapter 7. At last, nomenclature to explain symbols used in equations, preliminary work for next further extension of the theory are provided in Appendix A and B, and list of publications related to the present work is available in Appendix B.

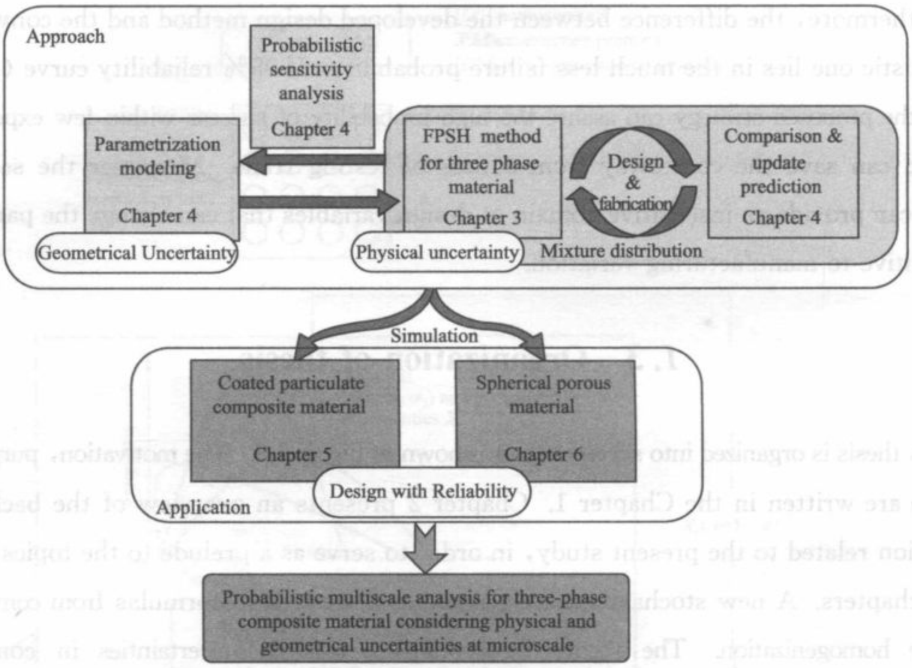

Fig. 1. 3. 1 Framework of this thesis

Chapter 2 Background and theoretical fundamentals

2.1 Micromechanics of composite material

The micro scale approach (micromechanics) is thought to be most suited for applications involving fabrication and material development, where an accurate evaluation of the microstresses and strains are critical; however, this detailed information often comes at analysis of structural components. In contrast, the macro scale approach (macromechanics) is clearly the more computationally efficient, thereby facilitating its use in large-scale component design and analysis; however, this efficiency may come at the cost of accuracy in comparison to its more computationally intense micro scale counterpart in Fig. 2.1.1, particularly when highly localized, non-uniform behavior relative to the representative volume element (RVE) dominates. Consequently, with these given considerations, a variety of micro scale and macro scale theoretical approaches continue to be pursued and refined in the literature with the ultimate goal of developing an approach that is both computationally efficient and accurate for deformation and damage analysis under general nonisothermal, multiaxial loadings. One of the main drawbacks of the macromechanical approach, as indicated in Table 2.1.1, is the requirement for an anisotropic constitutive theory (for most types of composites). In the linear elastic regime, this is not a major drawback, but in the presence of material nonlinearity, this requirement adds significantly to the model's theoretical and characterization complexity. Nevertheless, a number of anisotropic deformation models at the macro (or composite) level have been proposed.

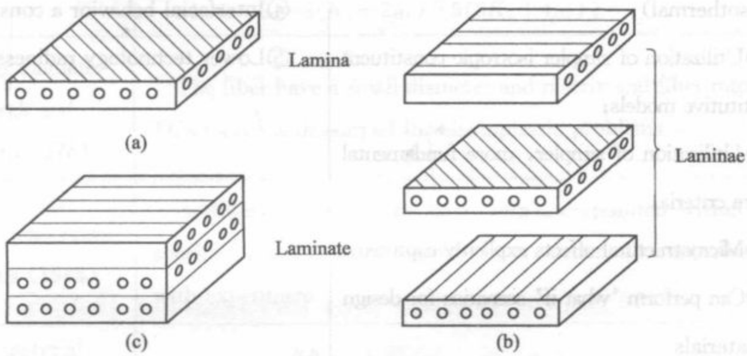

Fig. 2.1.1 Micro versus macro structure

Table 2.1.1 Comparison between micromechanics and macromechanics

	Advantages	Disadvantages
Macro-mechanical-nics	①Computational efficiency; ②Experimental testing incorporates all in-situ effects (interface, damage, residual stress, etc.); ③Aligned with standard ply-level design procedure; ④Tends towork well for: a. Fiber-dominated situations; b. Linear, isothermal regime	①Anisotropic constitutive theory required; ②Requires additional complexities to handle: a. Tension/compression b. Tertiary creep damage c. Multiaxiality interaction. ③Needs recalibration (retesting) for changes in: a. Architecture/layup b. Volume fraction c. Processing history (residual stresses) ④ Phenomenologically based: accounts for physics of all nonlinearity on the wrong scale; ⑤Mathematical form of internal state variable evolutionary law-usually sbased on monolithic materials; ⑥Adversely impacted with nonisothermal loading
Micro-mechanical-nics	①Enables the capturing of the physics of deformation and damage at a more fundamental scale; ②Captures varying in-situ non-proportional, multiaxial stress and strain state (iso/nonisothermal); ③Utilization of simpler isotropic constituent constitutive models; ④Utilization of simpler, more fundamental failure criteria; ⑤Microstructural effects explicitly captured; ⑥Can perform 'what if' scenarios for design of materials	①Increased computational expense; ②Need for constituent constitutive response (fiber/matrix) as well as composite testing for validation; ③Possible need to recalibrate for in-situ effects; ④Interfacial behavior a constant unknown; ⑤Lower technology radiness level (TRL)

Table 2.1.2 Types of micromechanics and its characteristics

Micromechanics	Characteristics
Voigt method(1887)	$\boldsymbol{C}^* = c_1\boldsymbol{C}^{(1)} + c_2\boldsymbol{C}^{(2)}$ rule of mixtures in terms of the volume-averaged stiffness of the individual phases
Reuss method(1929)	$\boldsymbol{S}^* = c_1\boldsymbol{S}^{(1)} + c_2\boldsymbol{S}^{(2)}$ rule of mixture in terms of the volume averaged effective compliance
Hill's theorem(1952)	$C^*_{ijkl} \leqslant \frac{1}{V}\int_V C_{ijkl}\,\mathrm{d}V$ $S^*_{ijkl} \leqslant \frac{1}{V}\int_V S_{ijkl}\,\mathrm{d}V$ this indicates that Voigt gives upper approximation, and Reuss gives lower approximation
Eshelby inclusion method (1957,1959)	$K^* = K_1 + c_2(K_2 - K_1)(A_2)_{kkmm}$ where $(A_2)_{kkmm} = \frac{4\mu_1 + 3K_1}{4\mu_1 + 3K_2}$
Composite spheres assemblage model[Hashin, 1962, for long fibers(cylinder), Concentric Cylinder Assemblage(CCA)]	$K^* = K_1 + \frac{c_2(K_2 - K_1)(3K_1 + 4\mu_1)}{3K_2 + 4\mu_1 + 3(K_1 - K_2)c_2}$ where $c_2 = (a/b)^3$ is the volume fraction of the spherical particles. But it is not possible to derive an expression for effective shear modulus from composite spheres model
Self-consistent scheme (1965)	$K^* = \frac{4(1-2c_2)(1-c_2)\mu}{(3-c_2)c_2}, \mu^* = \frac{3(1-2c_2)\mu_1}{(3-c_2)}$ for $0 < c_2 < 0.5$ The above results show that the self-consistent method does not provide realistic results at the vicinity of $c_2 = 1/2$ in the case of voids or $c_2 = 2/5$ in the case of rigid inclusions
Mori-Tanaka method(1973)	$K^* = K_1 + \frac{c_2(K_2 - K_1)K_1}{[(1-c_2)(K_2 - K_1)g_1 + K_1]}$ $\mu^* = \mu_1 + \frac{c_2(\mu_2 - \mu_1)\mu_1}{(1-c_2)(\mu_2 - \mu_1)\beta_1 + \mu_1}$ where $\beta_1 = 6(K_1 + 2\mu_1)/[5(3K_1 + 4\mu_1)]$
Vanishing fiber diameter model(Dvorak and Bahei-El-Din, 1978)	The fiber have a small diameter and matrix and fiber must deform equally. This model is developed for elastoplastic problems
Combined voigt and reuss approximations (1984)	Additional assumptions have been incorporated within the approach for specific classes of composites in order to improve the correlation with experiment
Strength of material (Murthy and Chamis, 1986)	$K^* = -\frac{\Delta p}{(\Delta V/V)}$ where Δp is the bulk stress, $\Delta V/V$ is the bulk strain

At the beginning of micromechanics study of composite material, there are many mathematical description to model the properties tested by experiment. Some of them are listed in Table 2. 1. 2. Some of them are still being used even today. The above table focused on spherical inclusions and voids for the sake of clarity and simplicity. The extension to continuous fibers can be found in Mura [Mura, 1982], and Aboudi [Aboudi, 1993; Aboudi, 2014] compares the effective properties of a continuously reinforced glass/epoxy composite system, plotted versus the reinforcement volume fraction V_f, as predicted by the analytical micromechanics methods discussed above. It shows that neither the Voigt nor Reuss assumption [Reuss, 1929] is correct: the implied Voigt stress are such that the tractions at phase boundaries would not be in equilibrium, while the implied Reuss strains are such that inclusions and matrix could not remain bonded. Note that Voigt and Reuss form that the upper and lower bounds for the effective stiffness (C_{ijkl}) tensor of the composite; however, when dealing with engineering constants, these will not always provide such bounds as evident from an examination of the transverse Poisson ratio, v_{23}. In the specific case of an ellipsoidal inclusion, the Eshelby equivalent inclusion principle [Eshelby, 1957] forms a means for the determination of the elastic field in the inclusion. From this solution for the ellipsoidal inclusion, many special cases such as sphere, elliptic cylinder, spheroid, crack, etc., can be derived. Furthermore, it is evident that only the Method of Cells (MOC) [Aboudi, 1986] and Mori-Tanaka [Mori, 1973] method are consistently within the tight bounds given by Concentric Cylinder Assemblage (CCA) [Hashin, 1962] for all stiffness properties (E_1, E_2, G_{12}, and G_{23}), whereas Vanishing Fiber Diameter model (VFD) [Dvorak, 1973], SOM (strength of materials) [Murthy, 1986], and Self-consistent Scheme (SCS) [Budiansky, 1965] are typically outside the Concentric Cylinder Assemblage (CCA) bounds that obviously within the Voigt and Reuss predictions. Also it is interesting to note that only for the case of E_2, v_{23}, and G_{23} do Method of Cells (MOC) and Mori-Tanaka (MT) differ noticeably. However, the popularity of the Mori-Tanaka (MT) method stems from the availability of simple closed-form expressions for the effective moduli, whereas MOC also has closed-form expressions, although they are slightly more involved. It should be remembered, however, that the MOC and its generalizations can be extended to any type of nonlinear material behavior without any inconsistencies or extra constraints.

2. 2 Homogenization and localization theory

Continuum mechanics is based on the concept of a homogeneous continuum, which can

此为试读，需要完整PDF请访问：www.ertongbook.com