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The 1st International Conference on Modeling and Simulation
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鄭州大學橡膠模具國家工程研究中心 主編



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第一届高聚物成型加工与材料物性预测 国际学术研讨会论文集

郑州大学橡塑模具国家工程研究中心 主编



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郑州大学橡塑模具国家工程研究中心 主编

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前 言

高聚物制品在国防、汽车、机械电子、石油化工、轻工等国家支柱产业及日常生活中得到广泛的应用。高聚物制品优良的物理、力学性质来源于材料的组分与不同层次和尺度的微结构；不同层次和尺度的微结构的形成和演化又依赖特殊的制备和加工技术。因此，只有多尺度分析方法才能实现高聚物成型过程及制品性能的宏、细、微观的动态耦合分析，了解成型过程中材料的微观结构演化历史，确定微观结构形态与最终制品宏观性能之间的科学定量关系，研究高聚物在成型过程的变化规律。

微观、多尺度问题的研究涉及材料学、聚合物加工、力学和计算机等学科，是当前聚合物加工领域最活跃的研究方向之一。为促进我国学者对该问题的深入研究，加强与国际同行的交流与合作，郑州大学橡塑模具国家工程研究中心在国家自然科学基金委员会的支持下，在重大项目“高聚物成型加工及模具设计中的关键力学和工程问题”承担单位协助下，结合该重大项目各子课题的研究进展，组织召开了“第一届高聚物成型加工与材料物性预测国际学术研讨会”。会议围绕材料物性的多尺度、成型过程中关键力学问题、工艺过程与制品质量控制、制品微观结构的演化机理和模具优化设计等专题进行研究和讨论。

来自美国、俄罗斯、英国、加拿大以及中国内地、中国台湾和中国香港等多个国家和地区享有盛名的专家、学者和业界同仁、专业技术杂志的主编等参加了这次会议，他们在多尺度建模、微观结构演化、制品质量控制等方面报告了世界上最新成果，分析了存在的问题和可能的解决方法，为今后该领域的发展指明了方向。

论文集收集了会议重要报告四十四篇，内容涉及多尺度研究的各个方向，有些还是世界上首次公开报告的成果，有重要学术价值。相信本次会议和论文集将会为我国聚合物加工的理论研究、产业化及技术创新起到积极的推动作用。

申长雨
2006. 10

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The Role, Development, and Prediction of Microstructure in Polymer Processing

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Polymer processing research provides the basis for developing a unified approach to dealing with polymer handling and transformation processes. It combines the principles of polymer science with the fundamentals of engineering and science to obtain useful polymeric products from optimized resins and manufacturing processes.

A typical polymer processing sequence starts with a solid (and sometimes liquid) resin in granular or powder form (random configuration), and ends with the transformation of the resin into a solid product with specified shape, dimensions, and short/long term properties under field conditions. The sequence of operations experienced by the material during this transformation involves solids transport, heating, melting, melt flow, shaping in a die or mold, and finally solidification, by cooling in the case of thermoplastics, or curing by heating in the case of thermosets. Thus, a variety of interactive and complex phenomena are involved, such as heat transfer, fluid flow, melting, solidification, chemical reactions, etc. These phenomena produce the thermo-mechanical history (temperature, velocity, deformation, and stress fields), that the polymer experiences during processing.

The thermo-mechanical history experienced by the polymer imparts to it a microstructure (crystallinity, morphology, orientation, residual stresses, etc.). This microstructure ultimately determines the properties of the final product (mechanical, optical, barrier, etc.). The field of polymer processing attempts to study and manipulate the interactions among the various components of the system: the resin, process, microstructure, and product properties. Computer simulation has been the tool of choice to achieve this objective.

Polymers exhibit complex rheological behavior, in both the molten and solid states. Furthermore, their thermal and thermodynamic properties are not readily available. Therefore, computer simulation requires extensive effort in the selection and determination of resin properties and constitutive models. Furthermore, in order to predict properties or microstructure, it is necessary to employ multi-scale models.

In spite of the above complexities, substantial progress has been made in the application of computer simulation to polymer processing. The presentation will review some of the recent developments in the field, with examples of research on microstructure development, characterization, and prediction in the areas of injection molding and film blowing.

Time-space Coupled Two-scale Method for the Heat Transfer Problem in Composite Material Structure With Periodicity

Youai Li, Junzhi Cui

Abstract: In this paper, a time-space coupled two-scale method is presented for the heat transfer problem of the structure of composite materials with periodic configurations, whose material coefficients generally depend on time t . At first, the main idea of time-space coupled two-scale method is briefly stated. The time-space coupled two-scale asymptotic expansion for the solution is given. And then the error estimation for the approximate solution with two-order terms is shown. Finally, the numerical example demonstrates the effectiveness of this method.

Keywords: Composite material with periodic configuration, Heat transfer problem, Time-Space Coupled Two-Scale Analysis, Homogenization

1 Introduction

In the last decade there is a rapidly growing interest in the multi-scale analysis of material sciences and engineering computations, it is because many of investigated problems involve multi-physics and multi-scale phenomena, and it is needed to capture both the macro-behavior and micro-behavior of them in practice. Several effective multi-scale methods can be found in literature, including the asymptotic expansion method with periodic boundary conditions of Lions and al^[1], the oscillating test functions method proposed by Tartar^[12,13], the asymptotic expansion method with Dirichlet boundary conditions due to Cui and Cao^[3~5], the multi-scale finite element method from Hou and al^[7], and the Heterogeneous multi-scale method (HMM hereafter) by E and Engquist^[6]. In particular, it can be concluded that the macro-behavior is accurately simulated by using these methods at least for some special problems, for instance, problems with scale separation. Up to now, most of studies on the multi scale analysis (hereinafter MSA) methods for the composite materials and their structures are concentrated on steady problems. A few of papers^[1,4] are concerned with the time dependent problems of composite materials with periodic configurations. By regarding the time t as a parameter, Cao^[2] and Ming and Zhang^[10] considered a class of the time dependent problems based on the two-scale homogenization method.

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In the present paper, we study the heat conduction problem for the structure of composite materials, whose material coefficients have ϵ -small periodicity with respect to space coordinates $x \in R^n$ and generally depend on time t . In order to effectively capture the microscopic variation of the structural behaviors with respect to space and time at the same time, we modify the conventional two-scale asymptotic analysis only in space to propose a time-space coupled two-scale analysis method for the heat conduction problem of composite material structure. We will discuss the well-posedness of the new method, and analyze its error. The numerical experiments show that our time-space coupled two-scale analysis method is valid.

The rest of this paper is organized as follows. The basic idea of the time-space coupled two-scale analysis method for the parabolic problem of the structure of composite materials with small periodicity is briefly introduced in section 2. In the third section, we show the time-space coupled two scale expansions. The error of finite terms approximate solution in the section 4 is given. Numerical result is given in section 5. The conclusions are given in the last section.

Denote uniformly by C the positive constant without distinction. For the sake of convenience, we use the Einstein summation convention on repeated indices. Throughout this paper, Q denotes the n -dimension unit cube.

2 Basic Idea of the Time-space Coupled Two-scale Analysis Method

In this paper, we consider the following heat conduction problem of the structure of composite materials with small periodicity.

$$\begin{aligned} \rho^\epsilon(x,t)c^\epsilon(x,t)\frac{\partial u^\epsilon(x,t)}{\partial t} - \frac{\partial}{\partial x_i} \left(k_{ij}^\epsilon(x,t)\frac{\partial u^\epsilon(x,t)}{\partial x_j} \right) \\ = f(x,t), (x,t) \in \Omega \times (0,T), \\ u^\epsilon(x,t) = g_b(x,t), (x,t) \in \partial\Omega \times (0,T) \\ u^\epsilon(x,0) = g_i(x), x \in \Omega \end{aligned} \quad (2.1)$$

where $\Omega \in R^n$ with n dimension space, $\rho^\epsilon(x,t)$ is the density function, $c^\epsilon(x,t)$ is the heat capacity function, and $k_{ij}^\epsilon(x,t)$ ($i, j=1, 2, \dots, n$) are the heat conduction coefficients, $f(x,t)$, $g_b(x,t)$ and $g_i(x)$ are given functions. From composite material sciences, it is well known that for the composite materials with small periodicity $\rho^\epsilon(x,t)$, $c^\epsilon(x,t)$ and $k_{ij}^\epsilon(x,t)$ ($i, j=1, 2, \dots, n$) have ϵ -small periodicity with respect to space coordinates x , where ϵ is the size of basic cells of the composite materials. It means that

$$\begin{aligned} \rho^\epsilon(x,t) &= \rho^\epsilon(x+\epsilon e_i, t), \\ c^\epsilon(x,t) &= c^\epsilon(x+\epsilon e_i, t), \\ k_{ij}^\epsilon(x,t) &= k_{ij}^\epsilon(x+\epsilon e_i, t), (i, j=1, 2, \dots, n) \end{aligned} \quad (2.2)$$

So they can be defined on a basic cell, hereafter each cell of investigated composite materials is denoted by ϵQ . Generally speaking, $\rho^\epsilon(x,t)$, $c^\epsilon(x,t)$ and $k_{ij}^\epsilon(x,t)$ ($i, j=1, 2, \dots, n$) depend on time t , but have not periodicity with respect to t . Let

$$\xi = \frac{x}{\epsilon} \quad (2.3)$$

$$\rho^\varepsilon(x, t) = \rho\left(\frac{x}{\varepsilon}, t\right), c^\varepsilon(x, t) = c\left(\frac{x}{\varepsilon}, t\right), k_{ij}^\varepsilon(x, t) = k_{ij}\left(\frac{x}{\varepsilon}, t\right), x \in \Omega \quad (2.4)$$

And the boundary condition $g_b(x, t)$ and initial condition $g_i(x)$ are given such that

$$g_b(x, 0) = g_i(x), x \in \partial\Omega$$

For convenience, we make the following assumptions:

(A1) $p(\xi, t)$, $c(\xi, t)$ and $k_{ij}(\xi, t)$ are 1-periodic functions with respect to ξ .

(A2) $\left\{k_{ij}\left(\frac{x}{\varepsilon}, t\right)\right\}$ is a symmetric matrix and satisfies the following uniformly elliptic condition:

$$\lambda |\eta|^2 \leq k_{ij}\left(\frac{x}{\varepsilon}, t\right) \eta_i \eta_j \leq \mu |\eta|^2, |\eta|^2 = (\eta_1^2 + \dots + \eta_n^2), \forall \eta \in R^n, \\ \left| \frac{\partial}{\partial t} k_{ij}\left(\frac{x}{\varepsilon}, t\right) \right| < \bar{\mu}, \forall (x, t) \in \Omega \times (0, T) \quad (2.5)$$

(A3) $\rho\left(\frac{x}{\varepsilon}, t\right)$, $c\left(\frac{x}{\varepsilon}, t\right)$ and $k_{ij}\left(\frac{x}{\varepsilon}, t\right) \in L^\infty(\Omega \times [0, T])$

(A4) there exist ρ_0 , ρ_m , c_0 and c_m such that

$$0 < \rho_0 \leq \rho\left(\frac{x}{\varepsilon}, t\right) \leq \rho_m, 0 < c_0 \leq c\left(\frac{x}{\varepsilon}, t\right) \leq c_m, \forall (x, t) \in \Omega \times (0, T)$$

From the theory of parabolic problems^[8,9,14], under these conditions it follows that there exists a unique solution to the problem (2.1).

It is well known that in numerical integration methods of parabolic problems with homogenous coefficients, the time interval $[0, T]$ is always partitioned into many subintervals $[t_p, t_{p+1}]$ ($p = 0, 1, \dots, P-1$), and the structure Ω into mesh domain Ω^h composed of finite nodes with the space size h in FE method or FD method. Then the heat transfer behavior on global $\Omega \times (0, T)$ is characterized by finite nodal values on Ω^h at P discretized time nodes. For the stability and convergence of the discretized equations, the time step $t_{p+1} - t_p$ and the space mesh size h should be designed in such a way that the usual CFL condition be satisfied. Since compared with the size L of the structure Ω , the size ε of the basic cell is very small for the structure of composite materials, then inside each cell εQ the heat transfer behaves in shorter period. Thus, in order to capture the heat transfer behaviors inside each $\varepsilon Q \times (0, T)$, a very fine partition should be used for both space and time. This in turn leads to very large scale computation.

In what follows, the two-scale analysis method for steady problem will be extended to develop a time-space coupled Two-Scale analysis Method (TSM) for solving the problem (2.1). The basic idea is as follows: from conventional numerical integration methods of parabolic problem, the time interval $[0, T]$ is still divided into many subintervals $[t_p, t_{p+1}]$ ($p = 0, 1, \dots, P-1$), and each basic cell εQ is taken as the smallest unit for the space homogenization, and then based on time-space homogenization on $\varepsilon Q \times [t_p, t_{p+1}]$ the macroscopic homogenization problem is constructed, and at the same time the microscopic cell problems are defined on $\varepsilon Q \times [t_p, t_{p+1}]$. Actually the latter are always transformed to 1-normalized problems defined on a time-space normalized domain $Q \times [0, 1]$. It means that the homogenization solution is evaluated on $\Omega \times (0, T)$ based on the space meshes with the size h_0 and time nodes t_p ($p =$

0, 1, ..., P), and the microscopic cell solutions are obtained by numerically solving the time-space 1-normalized problems defined on $\mathbf{Q} \times [0, 1]$.

Generally speaking, the size h_0 of space meshes is greater than ϵ and $\Delta t = t_{p+1} - t_p$ is greater than ϵ^2 . Taking into account the usual CFL condition for the FD method of parabolic equations, we will choose $\Delta t = \lambda \epsilon^2$ as the pace of the time integration in our time-space coupled two-scale asymptotic analysis below, where λ is a parameter introduced by

$$\lambda \epsilon^2 = T/P$$

In another words, we partition the interval $[0, T]$ into $P = [T/(\lambda \epsilon^2)]$ subintervals by introducing nodes t_0, t_1, \dots, t_p . Without losing generality, we suppose that $t_0 = 0$ and $t_p = T$.

Note that λ can be chosen according to homogenization parameter values $\hat{\rho}(t_p)$, $\hat{c}(t_p)$ and $\hat{k}_{ij}(t_p)$ ($i, j = 1, 2, \dots, n$), and the stability and accuracy of the discrete system.

3 Time-Space Coupled Two-Scale Expansions

This section briefly shows the time-space coupled two-scale analysis expansions of the temperature field for the problem (2.1).

Since the density function $\rho\left(\frac{x}{\epsilon}, t\right)$ and the heat capacity function $c\left(\frac{x}{\epsilon}, t\right)$ vary slowly in phase, it is supposed that in a time subinterval $[t_p, t_{p+1}]$ the coefficients $\rho(\xi, t)$, $c(\xi, t)$ are constants. They can be chosen as follows

$$\rho(\xi, t) = \rho_p(\xi) \quad (3.1)$$

$$c(\xi, t) = c_p(\xi) \quad (3.2)$$

Assume the heat conduction coefficients $k_{ij}\left(\frac{x}{\epsilon}, t\right)$ ($i, j = 1, 2, \dots, n$) as follows

$$\begin{aligned} k_{ij}^p(\xi, t) &= k_{ij}(\xi, t_p) + \frac{dk_{ij}}{dt} \Big|_{t=t_p} (t - t_p) \\ &+ \frac{d^2 k_{ij}}{dt^2} \Big|_{t=t_p} (t - t_p)^2 + R_{ij}^p(\xi, t) \end{aligned} \quad (3.3)$$

let

$$w_{ij}^p(\xi) = k_{ij}(\xi, t_p),$$

$$s_{ij}^p(\xi) = \frac{dk_{ij}}{dt} \Big|_{t=t_p},$$

$$r_{ij}^p(\xi) = \frac{d^2 k_{ij}}{dt^2} \Big|_{t=t_p},$$

then

$$k_{ij}^p(\xi, t) = w_{ij}^p(\xi) + s_{ij}^p(\xi)(t - t_p) + r_{ij}^p(\xi)(t - t_p)^2 + R_{ij}^p(\xi, t) \quad (3.4)$$

where $\rho_p(\xi)$, $c_p(\xi)$, $w_{ij}^p(\xi)$ and $s_{ij}^p(\xi)$, $r_{ij}^p(\xi)$, $R_{ij}^p(\xi, t)$ are all smooth functions of ξ , and defined on n -dimension unit cube.

Without lose of generality, we assume that

$$k_{ij}^p(\xi, t) = w_{ij}^p(\xi) + s_{ij}^p(\xi)(t - t_p) + r_{ij}^p(\xi)(t - t_p)^2 \quad (3.5)$$

for all $t \in (t_p, t_{p+1})$, $t - t_p = \lambda \epsilon^2 \tau$ ($\tau \in (0, 1)$).

In view of assumption (3.5), $k_{ij}(\xi, \tau)$, on $[t_p, t_{p+1}]$, can be written as

$$k_{ij}^p(\xi, \tau) = w_{ij}^p(\xi) + \lambda s_{ij}^p(\xi) \epsilon^2 \tau + \lambda^2 r_{ij}^p(\xi) \epsilon^4 \tau^2$$

Now we introduce the time-space coupled two-scale asymptotic expansion for the temperature field of the problem (2.1).

From formal calculation we conclude following theorems:

Theorem 3.1 The solution $u^\epsilon(x, t)$ of the problem (2.1) can be expressed in $\Omega \times [t_p, t_{p+1}]$ as

$$u^\epsilon(x, t) = u_p^0(x, t) + \sum_{l=1}^{\infty} \epsilon^l \sum_{\langle \alpha \rangle = l} N_{\alpha_1 \dots \alpha_l}^p(\xi, \tau) D_\alpha^l u_p^0(x, t) \quad (3.6)$$

where $\alpha = (\alpha_1, \dots, \alpha_l)$, $\langle \alpha \rangle = |\alpha_1| + \dots + |\alpha_l|$, $\alpha_j = 1, 2, \dots, n$, $j = 1, 2, \dots, l$, D_α^l denotes the usual derivative operator, and $u_p^0(x, t)$ defined on $\Omega \times [t_p, t_{p+1}]$ is a differentiable function with respect to variable (x, t) , and $N_{\alpha_1 \dots \alpha_l}^p(\xi, \tau)$ defined on $Q \times [0, 1]$ are the functions of variables $\xi = (\xi_1, \dots, \xi_n)$ and τ , they are determined as follows:

(1) For $l=1$, $N_{\alpha_1}^p(\xi, \tau)$ ($\alpha_1 = 1, 2, \dots, n$) are the solution of following problems

$$\begin{aligned} \lambda^{-1} \rho_p(\xi) c_p(\xi) \frac{\partial N_{\alpha_1}^p(\xi, \tau)}{\partial \tau} - \frac{\partial}{\partial \xi_i} \left(w_{ij}^p(\xi) \frac{\partial N_{\alpha_1}^p(\xi, \tau)}{\partial \xi_j} \right) \\ = \frac{\partial w_{i\alpha_1}^p(\xi)}{\partial \xi_i}, (\xi, \tau) \in Q \times [0, 1] \\ N_{\alpha_1}^p(\xi, \tau) \text{ is 1-periodic in } \xi, \int_Q N_{\alpha_1}^p(\xi, \tau) d\xi = 0 \\ N_{\alpha_1}^p(\xi, 0) = \begin{cases} 0, & \text{if } p=0, \\ N_{\alpha_1}^{p-1}(\xi, 1), & \text{if } p \geq 1, \xi \in \bar{Q} \end{cases} \end{aligned} \quad (3.7)$$

(2) From $N_{\alpha_1}^p(\xi, \tau)$, the homogenization coefficients $\hat{k}_{\alpha_1 \alpha_2}^p(\alpha_1, \alpha_2 = 1, 2, \dots, n)$ are evaluated in following formula

$$\hat{k}_{\alpha_1 \alpha_2}^p = \int_0^1 \left[\int_Q \left(w_{\alpha_1 \alpha_2}^p + w_{\alpha_2 j}^p \frac{\partial N_{\alpha_1}^p(\xi, \tau)}{\partial \xi_j} \right) d\xi \right] d\tau \quad (3.8)$$

(3) For $l=2$, $N_{\alpha_1 \alpha_2}^p(\xi, \tau)$ ($\alpha_1, \alpha_2 = 1, 2, \dots, n$) are the solution of following problem

$$\begin{aligned} \lambda^{-1} \rho_p(\xi) c_p(\xi) \frac{\partial N_{\alpha_1 \alpha_2}^p(\xi, \tau)}{\partial \tau} \\ - \frac{\partial}{\partial \xi_i} \left[w_{ij}^p(\xi) \frac{\partial N_{\alpha_1 \alpha_2}^p(\xi, \tau)}{\partial \xi_j} \right] - \frac{\partial}{\partial \xi_i} (w_{i\alpha_2}^p(\xi) N_{\alpha_1}^p(\xi, \tau)) \\ - w_{\alpha_2 j}^p(\xi) \frac{\partial N_{\alpha_1}^p(\xi, \tau)}{\partial \xi_j} - w_{\alpha_1 \alpha_2}^p(\xi) + \hat{k}_{\alpha_1 \alpha_2}^p = 0, (\xi, \tau) \in Q \times (0, 1) \end{aligned} \quad (3.9)$$

$N_{\alpha_1 \alpha_2}^p(\xi, \tau)$ is 1-periodic function with respect to ξ ,

$$\int_Q \rho_p(\xi) c_p(\xi) N_{\alpha_1 \alpha_2}^p(\xi, \tau) d\xi = 0,$$

$$N_{\alpha_1 \alpha_2}^p(\xi, 0) = \begin{cases} 0, & p=0, \\ N_{\alpha_1 \alpha_2}^{p-1}(\xi, 1), & \xi \in \bar{Q}, p \geq 1. \end{cases}$$

In the above formula, the weighted integration of $N_{\alpha_1 \alpha_2}^p(\xi, \tau)$ is 0, and the weighted function is $\rho_p(\xi) c_p(\xi)$.

(4) The $u_p^0(x, t)$ is defined as follows

$$\begin{aligned} |\rho_p(\xi) c_p(\xi)| \frac{\partial u_p^0(x, t)}{\partial t} - \hat{k}_{\alpha_1 \alpha_2}^p D_{\alpha_1 \alpha_2}^2 u_p^0(x, t) &= f(x, t), (x, t) \in \Omega \times (t_p, t_{p+1}) \\ \hat{k}_{\alpha_1 \alpha_2}^p &= \int_0^1 \int_Q w_{\alpha_{ij}}^p(\xi) \frac{\partial N_{\alpha_2}^p(\xi, \tau)}{\partial \xi_j} d\xi d\tau + \int_Q w_{\alpha_1 \alpha_2}^p(\xi) d\xi \\ |\rho_p(\xi) c_p(\xi)| &= \int_Q \rho_p(\xi) c_p(\xi) d\xi \end{aligned} \quad (3.10)$$

and the initial condition is

$$u_p^0(x, 0) = \begin{cases} g_i(x), & \text{if } p=0, \\ u_{p-1}^0(x, t_p), & \text{if } p \geq 1 \end{cases} \quad (3.11)$$

and the boundary condition is

$$u_p^0(x, t) = g_b(x, t), (x, t) \in \partial\Omega \times (0, T) \quad (3.12)$$

Now set

$$u^0(x, t) = u_p^0(x, t), \text{ as } (x, t) \in \Omega \times (t_p, t_{p+1}), p=0, 1, \dots, P-1 \quad (3.13)$$

Then $u^0(x, t)$ is defined on $\Omega \times [0, T]$ and satisfied the initial conditions and boundary conditions, called as the macroscopic homogenization solution of the problem (2.1).

The l -order cell problems ($l \geq 3$) involve the macro-scale and the micro-scale together. In practical computation, we only need to calculate the 1-order or 2-order asymptotic expansions. So in this paper, we only discuss the 2-order approximation of u^ε .

For the equation (3.9), set

$$\begin{aligned} V &= \{v \in H^1(Q) \mid v \text{ is 1-periodic function of } \xi, \int_Q \rho_p(\xi) c_p(\xi) v d\xi = 0\}, \\ H &= L^2(Q). \end{aligned}$$

We have the following results.

Theorem 3.2 There exists a unique solution to Problem (3.9).

Theorem 3.3 $\hat{k}_{\alpha_1 \alpha_2}^p$ ($\alpha_1, \alpha_2 = 1, 2, \dots, n$) are symmetric positive matrixes.

Theorem 3.4 The homogenization equation (3.10)~(3.12) and each cell problem (3.7) admit a unique solution.

4 The Approximate Solution of Time-space Coupled TSM and its Error Estimation

In this section, we show the approximate solution with four finite terms for the asymptotic expansions of time-space coupled TSM and its error estimation. As we have known, such an approximation is needed in the practical computation.

For brevity, denote

$$\begin{aligned}\rho_p &= \rho_p(\xi), \quad c_p = c_p(\xi), \\ w_{ij}^p &= w_{ij}^p(\xi), \quad s_{ij}^p = s_{ij}^p(\xi), \quad r_{ij}^p = r_{ij}^p(\xi), \\ N_a^p &= N_a^p(\xi, \tau), \quad u_p^0 = u_p^0(x, t).\end{aligned}$$

For the asymptotic expansions of time-space coupled TSM in previous section the second order approximation solution can be written as

$$u_2^\epsilon(x, t) = u_p^0 + \epsilon N_{a_1}^p D_{a_1}^1 u_p^0 + \epsilon^2 N_{a_1 a_2}^p D_{a_1 a_2}^2 u_p^0 \quad (4.1)$$

For $p=0, 1, \dots, P-1$, set

$$L_p^\epsilon = \rho_p c_p \frac{\partial}{\partial t} - \frac{\partial}{\partial x_i} \left(k_{ij}^p \frac{\partial}{\partial x_j} \right) \quad (4.2)$$

Applying the operator L_p^ϵ to $(u^\epsilon - u_2^\epsilon)(x, t)$, we obtain the coefficient of ϵ^{-1} , ϵ^0 , ϵ^1 , \dots of error equation, respectively, as follows.

The coefficient of ϵ^{-1} is

$$\begin{aligned}& -\lambda^{-1} \rho_p c_p \frac{\partial N_{a_1}^p}{\partial \tau} D_{a_1}^1 u_p^0 + \frac{\partial w_{ia_1}^p}{\partial \xi_i} \frac{\partial u_p^0}{\partial x_{a_1}} + \frac{\partial}{\partial \xi_i} \left(w_{ij}^p \frac{\partial N_{a_1}^p}{\partial \xi_j} \right) D_{a_1}^1 u_p^0 \\ & = \left\{ -\lambda^{-1} \rho_p c_p \frac{\partial N_{a_1}^p}{\partial \tau} + \frac{\partial w_{ia_1}^p}{\partial \xi_i} + \frac{\partial}{\partial \xi_i} \left(w_{ij}^p \frac{\partial N_{a_1}^p}{\partial \xi_j} \right) \right\} D_{a_1}^1 u_p^0\end{aligned} \quad (4.3)$$

Taking into account the equation (3.7), we obtain that the coefficient of ϵ^{-1} is zero.

The coefficient of ϵ^0 of the error equation satisfies

$$\begin{aligned}& f(x, t) - \rho_p c_p \frac{\partial u_p^0}{\partial t} - \left\{ \lambda^{-1} \rho_p c_p \frac{\partial N_{a_1 a_2}^p}{\partial \tau} - \frac{\partial}{\partial \xi_i} \left(w_{ij}^p \frac{\partial N_{a_1 a_2}^p}{\partial \xi_j} \right) \right. \\ & \left. - \frac{\partial}{\partial \xi_i} (w_{ia_2}^p N_{a_1}^p) - w_{a_1 i}^p \frac{\partial N_{a_2}^p}{\partial \xi_j} - w_{a_1 a_2}^p + \hat{k}_{a_1 a_2}^p \right\} D_{a_1 a_2}^2 u_p^0 + \hat{k}_{a_1 a_2}^p D_{a_1 a_2}^2 u_p^0 \\ & = f(x, t) - \rho_p c_p \frac{\partial u_p^0}{\partial t} + \hat{k}_{a_1 a_2}^p D_{a_1 a_2}^2 u_p^0 \\ & = 0\end{aligned} \quad (4.4)$$

So the error equation with second order approximation can be written as

$$L_p^\epsilon (u^\epsilon - u_2^\epsilon) = \epsilon F^\epsilon \quad (4.5)$$

where

$$\begin{aligned}F^\epsilon &= -\rho_p c_p N_{a_1}^p \frac{\partial D_{a_1}^1 u_p^0}{\partial t} - \epsilon^1 \rho_p c_p N_{a_1 a_2}^p \frac{\partial D_{a_1 a_2}^2 u_p^0}{\partial t} \\ & \quad + w_{ij}^p \left(N_{a_1}^p D_{a_1 ji}^3 u_p^0 + \frac{\partial N_{a_1 a_2}^p}{\partial \xi_j} D_{a_1 a_2 i}^3 u_p^0 \right) \\ & \quad + \epsilon w_{ij}^p N_{a_1 a_2}^p D_{a_1 a_2 ji}^4 u_p^0 \\ & \quad + \epsilon \lambda \tau s_{ij}^p \left(\frac{\partial^2 u_p^0}{\partial x_i \partial x_j} + \frac{\partial N_{a_1}^p}{\partial \xi_j} D_{a_1 a_2 i}^2 u_p^0 \right)\end{aligned}$$

$$\begin{aligned}
& +\varepsilon^2 \lambda \tau s_{ij}^p \left(N_{\alpha_1}^p D_{\alpha_1 j i}^3 u_p^0 + \frac{\partial N_{\alpha_1 \alpha_2}^p}{\partial \xi_j} D_{\alpha_1 \alpha_2 i}^3 u_p^0 \right) \\
& +\varepsilon^3 \lambda \tau s_{ij}^p N_{\alpha_1 \alpha_2}^p D_{\alpha_1 \alpha_2 j i}^4 u_p^0 \\
& +\varepsilon^3 \lambda^2 \tau^2 r_{ij}^p \left(\frac{\partial^2 u_p^0}{\partial x_i \partial x_j} + \frac{\partial N_{\alpha_1}^p}{\partial \xi_j} D_{\alpha_1 i}^2 u_p^0 \right) \\
& +\varepsilon^4 \lambda^2 \tau^2 r_{ij}^p \left(N_{\alpha_1}^p D_{\alpha_1 j i}^3 u_p^0 + \frac{\partial N_{\alpha_1 \alpha_2}^p}{\partial \xi_j} D_{\alpha_1 \alpha_2 i}^3 u_p^0 \right) \\
& +\varepsilon^5 \lambda^2 \tau^2 r_{ij}^p N_{\alpha_1 \alpha_2}^p D_{\alpha_1 \alpha_2 j i}^4 u_p^0 + \frac{\partial}{\partial \xi_i} (\tau w_{ij}^p N_{\alpha_1 \alpha_2}^p) D_{\alpha_1 \alpha_2 j}^3 u_p^0 \\
& +\lambda \tau \frac{\partial}{\partial \xi_i} s_{ij}^p \frac{\partial u_p^0}{\partial x_j} + \lambda \tau \frac{\partial}{\partial \xi_i} \left(s_{ij}^p \frac{\partial N_{\alpha_1}^p}{\partial \xi_j} \right) D_{\alpha_1}^1 u_p^0 \\
& +\varepsilon \lambda \tau \frac{\partial}{\partial \xi_i} (s_{ij}^p N_{\alpha_1}^p) D_{\alpha_1 j}^2 u_p^0 + \varepsilon \lambda \tau \frac{\partial}{\partial \xi_i} \left[s_{ij}^p \frac{\partial N_{\alpha_1 \alpha_2}^p}{\partial \xi_j} \right] D_{\alpha_1 \alpha_2}^2 u_p^0 \\
& +\varepsilon^2 \lambda \tau \frac{\partial}{\partial \xi_i} (s_{ij}^p N_{\alpha_1 \alpha_2}^p) D_{\alpha_1 \alpha_2 j}^3 u_p^0 + \varepsilon^2 \lambda^2 \tau^2 \frac{\partial r_{ij}^p}{\partial \xi_i} \frac{\partial u_p^0}{\partial x_j} \\
& +\varepsilon^2 \lambda^2 \tau^2 \frac{\partial}{\partial \xi_i} \left[r_{ij}^p \frac{\partial N_{\alpha_1}^p}{\partial \xi_j} \right] D_{\alpha_1}^1 u_p^0 + \varepsilon^3 \lambda^2 \tau^2 \frac{\partial}{\partial \xi_i} [r_{ij}^p N_{\alpha_1}^p] D_{\alpha_1 j}^2 u_p^0 \\
& +\varepsilon^3 \lambda^2 \tau^2 \frac{\partial}{\partial \xi_i} \left[r_{ij}^p \frac{\partial N_{\alpha_1 \alpha_2}^p}{\partial \xi_j} \right] D_{\alpha_1 \alpha_2}^2 u_p^0 \\
& +\varepsilon^4 \lambda^2 \tau^2 \frac{\partial}{\partial \xi_i} [r_{ij}^p N_{\alpha_1 \alpha_2}^p] D_{\alpha_1 \alpha_2 j}^3 u_p^0
\end{aligned} \tag{4.6}$$

The boundary condition is

$$(u^\varepsilon(x, t) - u_2^\varepsilon(x, t)) |_{\partial \Omega \times (t_p, t_{p+1})} = -\varepsilon N_{\alpha_1}^p D_{\alpha_1}^1 U_p^0 - \varepsilon^2 N_{\alpha_1 \alpha_2}^p D_{\alpha_1 \alpha_2}^2 U_p^0 \tag{4.7}$$

And the initial condition is

$$(u^\varepsilon(x, 0) - u_2^\varepsilon(x, 0)) = 0 \tag{4.8}$$

Define

$$B = H^1((0, T), H^4(\Omega)) \tag{4.9}$$

B is Banach space equipped with the following norm

$$\|u(x, t)\|_B^2 = \int_0^T (\|u(\cdot, t)\|_{H^4} + \|u'(\cdot, t)\|_{H^4})^2 dt, \forall u \in B \tag{4.10}$$

For the 2-order approximate solution $u_2^\varepsilon(x, t)$, we acquire the following error estimation:

Theorem 4.1 Assume that $u_p^0 \in H^1((0, T), H^4(\Omega))$ is the solution of the homogenization problem (3.10)~(3.13), $N_{\alpha_1}^p \in H^1((0, 1), w^{1, \infty}(Q))$ and $N_{\alpha_1 \alpha_2}^p(\xi, \tau) \in H^1((0, 1), w^{1, \infty}(Q))$, $\alpha_1, \alpha_2 = 1, \dots, n$, are the solutions of the unit cell problems in previous section, then the problem (4.5)~(4.8) has a unique solution $u^\varepsilon - u_2^\varepsilon$. Moreover, $(u^\varepsilon - u_2^\varepsilon) \in B$, and there exists a constant c , which only depends on $\lambda, \mu, \rho_0, \rho_m, c_0, c_m, \Omega$ and T , such that