Engineering Analysis with Boundary Elements 94 (2018) 172–183

Contents lists available at ScienceDirect

Engineering Analysis with Boundary Elements

journal homepage: www.elsevier.com/locate/enganabound

A Trefftz collocation method for multiple interacting spherical nano-inclusions considering the interface stress effect

Leiting Dong[a], Junbo Wang[a], Peng Yan[a,*], Zaoyang Guo[b,*]

[a] School of Aeronautic Science and Engineering, Beihang University, Beijing 100191, China
[b] School of Science, Harbin Institute of Technology, Shenzhen, Guangdong 518055, China

ARTICLE INFO

Keywords:
Trefftz collocation method
Spherical harmonics
Interface stress effect
Generalized Young-Laplace equations

ABSTRACT

In this study, a Trefftz collocation method (TCM) is proposed for modeling multiple interacting nano-scale spherical inhomogeneities considering the interface stress effect. The Papkovich–Neuber (P–N) general solutions are used as Trefftz trial functions, which are expressed in terms of spherical harmonics. Non-singular harmonic functions, and singular harmonics from multiple source points are included, facilitating the study of multiple inclusions. Characteristic lengths are used to scale the Trefftz trial functions, to avoid ill-conditioning of the derived system of linear equations. The collocation method is used to enforce boundary conditions. The displacement continuity and the stress jump across the matrix/inclusion interface, which is described by the generalized Young–Laplace equation for solids, are also enforced by the collocation method. Numerical results by the proposed Trefftz method agree well with the available analytical solutions in the literature. The stress distributions of solids containing nano-inhomogeneities show significant size-dependency, in contrast to those for composites without considering the interface stress effect. Interactions of multiple nano-inclusions are also studied, which can be used as benchmark solutions in future studies.

1. Introduction

Composites with nanosized reinforcements, such as nanoparticles and nanofibers, etc., have been widely used in various engineering practices. Nanocomposites usually demonstrate very different material properties as compared to composites with micro-sized reinforcements, part of which can be attributed to the interface effects. Thus a good understanding of interface effects in nanocomposites, and establishing effective analytical/numerical nano-mechanical models where interface effects are considered, will be much beneficial for the design and development of nanocomposites.

Various models, such as the free sliding model [1], the linear spring model [2], the dislocation-like model [3], the interphase model [4], the interface stress model [5–12] etc., are used to simulate the mechanical properties of interfaces in composites. Among these models, the interface stress model has attracted much attention. The concept of interface stress in solids was first introduced by Gibbs [10] and have been extensively investigated since Gurtin and Murdoch [11,12] incorporated interface stress into continuum mechanics. In the Gurtin–Murdoch model, the interface is considered as a negligibly thin layer adhering to bulk materials without slipping. The stress jump across the interface is equal to the surface divergence of the interface stress, which is described by the generalized Young–Laplace equations.

Attempts have been made by researchers to find analytical solutions for nanocomposites considering the interface stress effect. For problems with a single nano-inhomogeneity, Tian [13] obtained the analytical solution for the elastic field of a nanoscale 2D circular inhomogeneity in an infinite matrix under arbitrary remote loading and a uniform eigenstrain, by using the complex potential technique of Muskhelishvili; Duan et al. [7], He and Li [14], Lim et al. [15], Sharma et al. [16], etc. provided analytical expressions of an embedded 3D spherical nano-inhomogeneity with the help of the Papkovitch–Neuber displacement potentials. Duan et al. [9], Chen et al. [17], etc. also extended the Eshelby tensor and the Eshelby formalism to nano-inhomogeneities in order to predict the effective material properties of nanocomposites and nanoporous materials, where the interactions among inhomogeneities are neglected.

However, little literature is available on problems of multiple interacting nano-inhomogeneities considering the Gurtin–Murdoch interface model, most of which focuses on 2D problems. For example, Zhang and Shen [18] adopted series expansion in bipolar coordinates to investigate the effects of surface energy on the interaction between holes or the edge; Mogilevskaya et al. [19,20] investigated stress distribution of

* Corresponding authors.
E-mail addresses: yanpeng117@buaa.edu.cn (P. Yan), z-guo@foxmail.com (Z. Guo).

https://doi.org/10.1016/j.enganabound.2018.07.002
Received 14 February 2018; Received in revised form 3 June 2018; Accepted 2 July 2018
Available online 20 July 2018
0955-7997/

multiple interacting circular nano-inhomogeneities or/and nano-pores. A semi-analytical method is used to obtain elastic fields in their work, and the results show that the interaction among nano-inhomogeneities can be scarcely neglected. Based on Mogilevskaya's work, Kushch et al. [21,22] presented semi-analytical solutions of the problems containing multiple spherical inhomogeneities with surface effects described by the complete Gurtin–Murdoch model. For 3D problems of multiple interacting nano-inhomogeneities considering the interface stress effect, it is nearly impossible to find analytical solutions due to mathematical complexities.

The difficulty in finding analytical solutions for multiple interacting nano-inhomogeneities problems promoted the development of numerical tools. Chen et al. [17] and Tian and Rajapakse [23] developed a kind of surface element to take into account the surface/interface stress effect based on the Gurtin–Murdoch theory. Feng et al. [24] developed 3D FEM with the surface stress effect to investigate the elastic properties of silicon nanowires. In addition, a boundary element method (BEM) is proposed by Dong and Pan [25] to analyze the stress field in nano-inhomogeneities considering surface/interface effects.

In order to facilitate the study of multiple 3D interacting nano-inhomogeneities problems, in this study we develop a 3D Trefftz method by employing the Papkovich–Neuber (P–N) solutions that automatically satisfy Navier's equations. The P–N potentials are expressed in terms of spherical harmonics, including both non-singular and singular terms. The boundary conditions are enforced through the collocation technique, where the P–N solutions are matched to the displacement or traction boundary conditions point by point. The displacement continuity and the stress jump across the matrix/inclusion interface, which is described by the generalized Young–Laplace equation for solids, are also enforced by the collocation method. However, the system of equations established by the Trefftz method is often severely ill-conditioned, especially for 3D Trefftz solutions in terms of spherical harmonics [26,27]. In this study, characteristic lengths are used to scale the Trefftz trial functions, so the condition number of the equations will be significantly reduced and the accuracy of the numerical solution can be guaranteed. Finally, several numerical examples are presented to verify the accuracy and stability of the present TCM. Numerical results of multiple interacting nano-inclusions are also given, which can be used as benchmark solutions in future studies.

The rest of this paper is organized as follows: in Section 2, the governing equations for multiple embedded 3D nano-inclusions are briefly reviewed. In Section 3, the Trefftz Collocation Method is given in detail. In Section 4, several examples are presented to verify the accuracy of the proposed method, and interactions of multiple nano-inclusions are studied. In Section 5, we complete this paper with some concluding remarks.

2. The governing linear elasticity equations for multiple 3D nano-inclusions

As shown in Fig. 1, solutions of 3D linear elasticity for the matrix and inclusions should satisfy the equations of stress equilibrium, strain displacement-gradient compatibility, as well as the constitutive relations in each domain Ω^k:

$$\nabla \cdot \boldsymbol{\sigma}^k + \mathbf{f}^k = 0 \tag{1}$$

$$\boldsymbol{\varepsilon}^k = \frac{1}{2}(\nabla \mathbf{u}^k + (\nabla \mathbf{u}^k)^*) \tag{2}$$

$$\boldsymbol{\sigma}^k = \lambda^k \mathrm{tr}(\boldsymbol{\varepsilon}^k)\mathbf{I}_3 + 2\mu^k \boldsymbol{\varepsilon}^k \tag{3}$$

where the superscript $k=0$ denotes the matrix material, and $k=1$, 2, 3… denotes multiple inclusions respectively. $\mathbf{u}^k$, ε^k, σ^k are stresses, strains, and displacements in matrix/inclusions. $\mathbf{f}^k$ is the body force in matrix/inclusions, which can be neglected for micromechanics

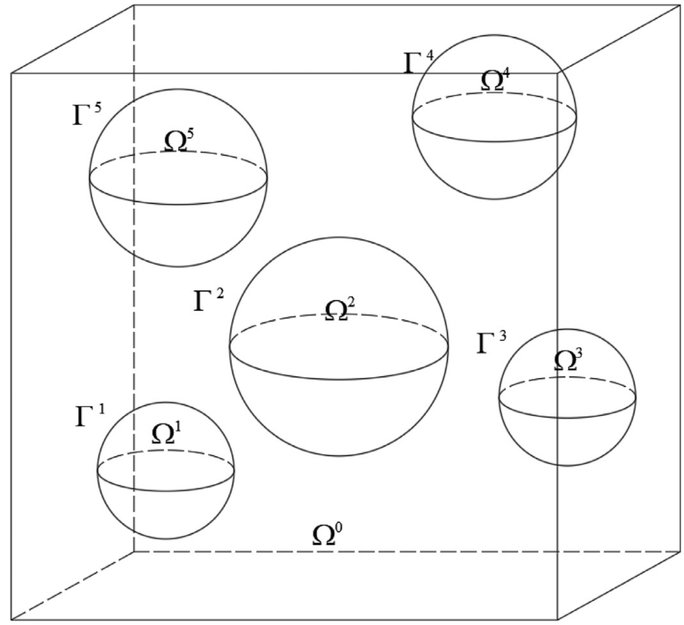

Fig. 1. An illustration of a matrix containing multiple inclusions.

of composites. $\nabla \cdot$ and $\nabla$are the divergence and gradient operators. $\lambda^k = \frac{\nu^k E^k}{(1-2\nu^k)(1+\nu^k)}$ and $\mu^k = \frac{E^k}{2(1+\nu^k)}$ are Lamé constants for matrix/inclusions, where E^k and ν^k are Young's modulus and Poisson's ratio. $\mathbf{I}_3$ is the 3D unit tensor and $\mathbf{I}_3 = \mathbf{e}_r \otimes \mathbf{e}_r + \mathbf{e}_\theta \otimes \mathbf{e}_\theta + \mathbf{e}_\varphi \otimes \mathbf{e}_\varphi$ in spherical coordinates, where $\mathbf{e}_r$, $\mathbf{e}_\theta$, $\mathbf{e}_\varphi$ are base vectors. $\mathrm{tr}(\varepsilon^k)$ denotes the trace of the strain tensor.

The boundary conditions can be written as:

$$\mathbf{u}^0 = \bar{\mathbf{u}} \quad \text{at } S_u \tag{4}$$

$$\mathbf{n} \cdot \boldsymbol{\sigma}^0 = \bar{\mathbf{t}} \quad \text{at } S_t \tag{5}$$

where $\bar{\mathbf{u}}$ and $\bar{\mathbf{t}}$ are the prescribed boundary displacements and boundary tractions at the displacement boundary S_u and the traction boundary S_t of the domain Ω^0, respectively.

The interface between the matrix and each inclusion has its own Lamé constants λ^s and μ^s, and its elastic response is governed by:

$$\left(\boldsymbol{\sigma}^0 - \boldsymbol{\sigma}^k\right) \cdot \mathbf{n} = -\nabla_s \cdot \boldsymbol{\tau}^s \quad \text{at } \Gamma^k \tag{6}$$

$$\mathbf{u}^0 = \mathbf{u}^k = \mathbf{u}^s \quad \text{at } \Gamma^k \tag{7}$$

$$\boldsymbol{\tau}^s = 2\mu^s \boldsymbol{\varepsilon}^s + \lambda^s \mathrm{tr}(\boldsymbol{\varepsilon}^s)\mathbf{I}_2 \tag{8}$$

$$\boldsymbol{\varepsilon}^s = \frac{1}{2}\left[D\mathbf{u}^s + (D\mathbf{u}^s)^*\right] \tag{9}$$

where $\mathbf{u}^s$, $\boldsymbol{\varepsilon}^s$ and $\boldsymbol{\tau}^s$ are interface displacement, strains and stresses, respectively. $\nabla_s = (\mathbf{I}_3 - \mathbf{nn}) \cdot \nabla$ is the gradient operator defined on the interface where $\mathbf{n}$ is the unit outer-normal vector of the interface. The operator D is defined so that $D\mathbf{u}^s = (\mathbf{I}_3 - \mathbf{nn}) \cdot (\nabla_s \mathbf{u}^s)$. $\mathbf{I}_2$ is the unit tangent tensor defined on the interface and $\mathbf{I}_2 = \mathbf{e}_\theta \otimes \mathbf{e}_\theta + \mathbf{e}_\varphi \otimes \mathbf{e}_\varphi$ in spherical coordinates. Eq. (6) is the generalized Young–Laplace equation for solids. Detailed discussions about the generalized Young–Laplace equation can be found in [5–9,11,12,28].

For the interface between the matrix and a spherical inclusion as shown in Fig. 2, $\boldsymbol{\varepsilon}^s$ and $\nabla_s \cdot \boldsymbol{\tau}^s$ can be expressed in spherical coordinates