Equivalent modulus of nanoporous materials based on Steigman-Ogden surface model

Chenyi Zheng (zheng_cy1@hdec.com)
Huadong Engineering Corporation Limited

Gaohui Li
Huadong Engineering Corporation Limited

Mengjie Zhang
Huadong Engineering Corporation Limited

Yali Jiang
Huadong Engineering Corporation Limited

Hongzhen Wang
Huadong Engineering Corporation Limited

Zhengliang Li
Huadong Engineering Corporation Limited

Mengcheng Sun
Huadong Engineering Corporation Limited

Haolei Zheng
Huadong Engineering Corporation Limited

Article

Keywords:

Posted Date: August 21st, 2023

DOI: https://doi.org/10.21203/rs.3.rs-3176965/v1

License: This work is licensed under a Creative Commons Attribution 4.0 International License. Read Full License

Additional Declarations: No competing interests reported.
Equivalent modulus of nanoporous materials based on Steigman-Ogden surface model

Chenyi Zheng\textsuperscript{1,\*}, Gaohui Li\textsuperscript{1}, Mengjie Zhang\textsuperscript{1}, Yali Jiang\textsuperscript{1}, Hongzhen Wang\textsuperscript{1}, Zhengliang Li\textsuperscript{1}, Mengcheng Sun\textsuperscript{1}, and Haolei Zheng\textsuperscript{1}

\textsuperscript{1}Huadong Engineering Corporation Limited, China, Hangzhou, Zhejiang 311122, China
\*Corresponding:zheng\_cy1@hdec.com

ABSTRACT

The work of this paper mainly includes two parts. The first part is to simplify the stress boundary equation of the complex Steigmann-Ogden surface model expressed by the surface gradient operator in spherical coordinates to the stress boundary equation expressed by the spatial gradient operator according to the surface projection tensor. This simplification can directly substitute the complex formula into the fingermark method and directly calculate it into the sizeable mathematical calculation software. In the second part, based on the Mori-Tanaka hole model, the displacement field is decoupled into a hydrostatic and partial displacement field. Based on the homogenization approach, the equivalent elastic modulus of nanoporous materials is solved by satisfying the displacement boundary equation on the boundary of the representative volume element (RVE). The hydrostatic displacement field corresponds to the macroscopic equivalent bulk modulus, while the offset displacement field corresponds to the macroscopic equivalent shear modulus. Finally, this paper conducted auspicious numerical experiments on various surface elastic parameters and explored their control mechanisms. The research in this paper can provide a theoretical basis for designing and manufacturing nanoporous materials.

1 Introduction

Nanoporous materials have numerous advantages due to their unique properties at the nanoscale. Some key advantages are: (a) Large surface area: Nanoporous materials have a high surface area-to-volume ratio, making them ideal for adsorption and catalysis applications. (b) Tailorable pore size and distribution: The size and distribution of the pores in nanoporous materials can be controlled during synthesis, allowing for precise tuning of their properties. (c) Enhanced mechanical and thermal properties: The small pore size in nanoporous materials leads to enhanced mechanical and thermal properties, making them ideal for applications where strength and durability are required. (d) Selective adsorption: Nanoporous materials can selectively adsorb molecules based on their size, shape, and chemical properties, making them useful for separation and purification applications. Overall, nanoporous materials offer a wide range of advantages and have the potential to revolutionize various fields such as energy, environmental science, biomedicine, and electronics.\textsuperscript{1-3}

Due to the superior properties of nanoporous materials, related research articles have also been developed, including the study of effective modulus\textsuperscript{4,5}, elastic response\textsuperscript{6-9} and strength analysis of nanoporous materials\textsuperscript{1,2,10,11}.

Scholars have tried to use the classical continuum mechanics theory to describe the mechanical behavior of nanoporous metal materials. Gurtin and Murdoch\textsuperscript{12} established the famous Gurtin-Murdoch surface mechanics model based on the conservation of linear and angular momentum of surface stress. Based on the variational principle and energy method, Sharma et al.\textsuperscript{13} analyzed the stress distribution inside and outside the nano-spherical cavity and inclusion. He and Li\textsuperscript{14} solved the displacement and stress components in the infinite elastic domain embedded in the nano-view hole. Kushch et al.\textsuperscript{15} used the potential displacement function in spherical coordinates to analyze the elastic interaction between multiple nano-spherical inclusions. In addition to the infinite elastic body, the Gurtin-Murdoch surface mechanical model has also been used to analyze the stress around spherical nano-void holes and nano-inclusions in the semi-infinite domain. In these documents, all parameter studies have revealed the strong size dependence of the stress field.

In addition to the stress analysis around nano-void and nano-inclusion, calculating effective elastic modulus is another area of interest for scholars. In the composite sphere assembly model framework, the Mori-Tanaka model and generalized self-consistent model, Duan et al.\textsuperscript{4} solved the equivalent bulk modulus and equivalent shear modulus of the element containing spherical inclusion under the axisymmetric condition. When the spherical inclusion’s bulk and shear modulus are reduced to zero, the equivalent modulus of the element containing a spherical hole can be obtained. Chen et al.\textsuperscript{16} calculated the equivalent elastic modulus of nanoporous components considering Gurtin-Murdoch surface mechanical model under axial symmetric load, transverse shear, and anti-plane shear. Duan et al.\textsuperscript{5} further developed a unified theoretical framework for predicting the
Considered a limited number of spherical particles in each crystal cell and analyzed the stress distribution and effective stiffness tensor of periodic particle reinforced nano-composite. Based on the conformal mapping in the complex variable function, Doan et al. determined the equivalent mechanical properties of two-dimensional composites containing arbitrary shape nano-void holes. The above documents are based on the macroscopic elastic solutions of nanoporous metals obtained from the Gurtin-Murdoch surface mechanical model, but Steigmann and Ogden pointed out that the Gurtin-Murdoch surface mechanical model only considers the resistance of the solid surface to surface tension and strain deformation, but completely ignores the bending stiffness of the solid surface. That is to say, it is impossible to deal with the stress state when the solid surface is subjected to compression or bending deformation. For this reason, the Steigmann–Ogden surface mechanics model that can consider the effect of bending stiffness is proposed. Therefore, considering the surface stiffness, it is necessary to provide a solution to the equivalent elastic modulus of nanoporous materials. Based on the displacement component function, the Steigmann-Ogden stress boundary equation is simplified by index notation. Then the homogenization approach solves the equivalent elastic volume and shear modulus of nanoporous materials.

The remainder of this paper is structured as follows. In section 2, the stress boundary condition equation of the Steigmann-Ogden surface model is simplified by index notation, and the influence of the surface gradient operator is eliminated. In addition, based on the displacement component function, the equivalent bulk modulus and equivalent shear modulus of nanoporous materials are calculated by the homogenization approach. In Section 3, extensive parametric studies are conducted to examine the effects of nanopore radius, surface stress parameters, surface bending parameters, and porosity on the equivalent elastic modulus of nanoporous materials. Finally, in Section 4, concluding remarks are made.

## 2 Method of solution

![Image](image1.png)

**Figure 1.** Internal structure of nanoporous materials and representative volume elements considering surface elasticity of pores

As shown in Fig. 1, the interior of nanoporous metal materials usually contains numerous nano-sized holes. These holes are assumed to have the same radius and are sparsely distributed, with no interaction. Therefore, the effect of each hole on the macroscopic mechanical properties of nanoporous metal materials can be regarded as equivalent. A concentric spherical unit around any hole is used as a representative volume element (RVE) for analysis, as shown in the right sub-figure of 1. The hole’s radius is \(a\), while the outer boundary radius of the RVE is \(b\), and \(b \gg a\). Therefore, the volume fraction (porosity) of RVE is \(f = a^3/b^3\). Through the above analysis and simplification, the current RVE model is consistent with the famous Mori-Tanaka hole model, that is, considering the constant positioning displacement field \(u\) acting on the infinite elastic outer boundary containing a single hole, the corresponding strain field is \(E\).

### 2.1 Improved boundary equation of Steigmann-Ogden surface/interface model

As the Gurtin-Murdoch surface elasticity model ignores the flexural resistance of solid surfaces, the surface elastic potential energy of solid surfaces, which may undergo significant curvature changes during loading and balancing, depends to a large extent on their curvature changes. For this reason, based on the Gurtin-Murdoch model, Steigmann and Ogden take into account the influence of curvature change of solid surface on surface elastic potential. Without considering the effect of surface tension, the stress boundary conditions at the cross-solid interface can be expressed as:

\[
[\sigma] \cdot n = \nabla_S \cdot \tau + \nabla_S \cdot ((\nabla_S \cdot M) n) - (\nabla_S \cdot n) \cdot (\nabla_S \cdot M)n,
\]  

(1)
where $\nabla_S$ and $\mathbf{M}$ represent surface gradient differential operators and surface bending moment tensors, respectively. The surface elastic constitutive relation in the Steigmann-Ogden model of surface elasticity is:

$$
\tau_{ij} = \lambda_0 e_{ij}^0 \delta_{ij} + 2\mu_0 e_{ij}^f, \quad M_{ij} = \zeta_0 \kappa_{ij} T_{ij} + 2 \chi_0 \kappa_{ij},
$$

(2a-b)

where $\zeta_0$ and $\chi_0$ represent the surface bending modulus and the surface curvature change tensor is equal to the symmetric part of the surface gradient of the surface slope change vector:

$$
\kappa_{ij} = -T_{ik} T_{jl} \vartheta_{kl},
$$

(3)

The vector of surface slope change is determined by the surface displacement:

$$
\vartheta_i = T_{ij} n_k u_{k,j}.
$$

(4)

Due to the existence of the surface gradient differential operator ($\nabla_S$), the calculation of surface stress boundary conditions (1) in the Steigmann-Ogden model is complicated. In order to solve this problem better, this paper simplifies the surface stress boundary conditions based on index notation and tries to use the surface projection tensor and spatial gradient differential operator to replace the surface gradient operator. First, the gradient operation is divided into the normal direction and surface direction by projection tensor:

$$
\frac{\partial}{\partial x_j} = N_{ij} \frac{\partial}{\partial x_i} + T_{ij} \frac{\partial}{\partial x_i},
$$

(5)

Here, the surface gradient differential operator ($\nabla_S$) is written as $T_{ij} \frac{\partial}{\partial x_i}$ in the indicator notation. Using the above equation, the surface stress boundary conditions (1) of the Steigmann-Ogden surface elasticity model can be transformed into:

$$
[\sigma]_{ij} n_i = \tau_{ij} + T_{ia} (M_{kl,n_j})_{a} - T_{ik} n_i n_i M_{ml, mn} n_j.
$$

(6)

On the boundary of a circular hole with radius $a$, its projection tensor and normal gradient tensor are respectively:

$$
\mathbf{T} = \mathbf{e}_\varphi \mathbf{e}_\varphi + \mathbf{e}_\theta \mathbf{e}_\theta, \quad \nabla n = \frac{1}{a} \mathbf{e}_\varphi \mathbf{e}_\varphi + \frac{1}{a} \mathbf{e}_\theta \mathbf{e}_\theta.
$$

(7,b)

Therefore, it is not difficult to find that the two-point product of projection tensor and normal gradient tensor is:

$$
T_{ik} n_{i,k} = \frac{2}{a}.
$$

(8)

Therefore, the equation (6) can be further simplified to:

$$
[\sigma]_{ij} n_i = \tau_{ij} + T_{ia} (M_{kl,n_j})_{a} - \frac{2}{a} M_{ml, mn} n_j.
$$

(9)

According to the index notation given by the above formula, the tensor expression of the stress boundary condition (1) can be given:

$$
[\sigma] \cdot n = \nabla \cdot \tau + \text{tr}\left( \left( \nabla (\nabla \cdot \mathbf{M}) \right) \cdot \mathbf{T} \right) n + \frac{1}{a} (\mathbf{I} - 3 \mathbf{N}) \cdot (\nabla \cdot \mathbf{M}).
$$

(10)

Compared with the original surface stress boundary condition (1) of the Steigmann-Ogden surface elasticity model, the simplified surface stress boundary condition no longer contains the surface gradient differential operator. However, it is represented by spatial gradient, surface projection tensor, and normal projection tensor. Because all the tensors are transformed into three-dimensional space instead of the spherical surface, it is easy to substitute them into computational mathematics software for a solution directly.

### 2.2 Calculation of equivalent bulk modulus of the RVE

This section is dedicated to solving the equivalent bulk modulus of spherical RVE shown in the right sub-figure of figure 1. In order to make the derivation results more general and applicable, it is advisable to replace the holes in RVE with inclusions first and then reduce the inclusions into holes after calculating the equivalent bulk modulus of RVE containing inclusions to obtain
the equivalent bulk modulus of spherical RVE containing holes. Now it is assumed that the macroscopic strain field acting on the outer boundary of RVE-containing inclusions has the following spherically symmetric form:

\[
E = \begin{bmatrix}
E_m & 0 & 0 \\
0 & E_m & 0 \\
0 & 0 & E_m
\end{bmatrix}.
\]

(11)

This represents that the RVE is in hydrostatic stress and strain, so the deformation mode is simple isotropic expansion or contraction. Under the action of spherically symmetric macroscopic strain, because there is no shear deformation, it is very convenient to calculate the equivalent bulk modulus of RVE directly. Without losing generality, it is assumed that the inclusion and matrix of spherical RVE have the following spherically symmetric displacement fields, respectively:

\[
u_R^1 = F_1 R + G_1 \frac{a^3}{R^2}, \quad u_R^1 = u_R^1 = 0,
\]

(12a,b)

\[
u_R^2 = F_2 R + G_2 \frac{a^3}{R^2}, \quad u_R^2 = u_R^2 = 0,
\]

(12c,d)

The superscript 1 and 2 represent the inclusion and matrix, respectively, and the corresponding local strain field can be obtained through the geometric relationship:

\[
\varepsilon_{ij}^1 = \frac{1}{2} \left( u_{i,j}^1 + u_{j,i}^1 \right), \quad \varepsilon_{ij}^2 = \frac{1}{2} \left( u_{i,j}^2 + u_{j,i}^2 \right).
\]

(13a,b)

Then the stress field in the inclusion and matrix can be obtained through the general Hooke's law:

\[
\sigma_{ij}^1 = \lambda_1 \varepsilon_{kk} \delta_{ij} + 2 \mu_1 \varepsilon_{ij}, \quad \sigma_{ij}^2 = \lambda_2 \varepsilon_{kk} \delta_{ij} + 2 \mu_2 \varepsilon_{ij},
\]

(14a,b)

where \( \lambda_{1,2} \) and \( \mu_{1,2} \) is the Lame constant. According to the relationship between elastic moduli, the bulk modulus is defined as \( \kappa_{1,2} = (3 \lambda_{1,2} + 2 \mu_{1,2})/3 \).

It is noted that there are four unknown coefficients in the radial displacement components of the inclusion and the matrix, so four boundary conditions need to be established to solve. First of all, the displacement condition shall be satisfied on the outer boundary of the inclusion RVE:

\[
u_R^2 |_{R=b} = E_m b.
\]

(15)

Secondly, considering that the displacement of the inclusion center cannot be singular, the coefficient \( G_1 \) must be zero:

\[G_1 = 0.
\]

(16)

Then, at the interface between the inclusion and the matrix, the radial displacement component shall meet the continuity condition:

\[u_R^1 |_{R=a} = u_R^2 |_{R=a}.
\]

(17)

Finally, consider the stress boundary condition (ref eqn3. mean-b) of the interface between the inclusion and the matrix. Under the action of the macro strain field given in the formula (ref eqn3. operate16), the change vector of the surface slope is zero:

\[\vartheta_i = T_{ij} n_k u_{k,j} = 0.
\]

(18)

It can be judged that the surface curvature modification tensor is also zero. Therefore, for the hydrostatic stress-strain state, the surface bending moment will not affect the surface stress boundary condition:

\[\sigma |_{ij} n_i = \tau_{ij}.\]

(19)

This surface stress boundary condition is entirely equivalent to the corresponding condition of the Gurtin-Murdoch surface elasticity model. Therefore, it can be predicted that the equivalent bulk modulus of RVE with inclusions or holes is independent of the surface bending stiffness.

Through the above four conditions (15, 16, 17 and 19), the four unknown coefficients \( F_1, F_2, G_1 \) and \( G_2 \) contained in the shift field can be uniquely located.
According to the homogenization principle, the average strain can be defined as\(^4\) according to the volume average method:

\[
\bar{\varepsilon}_{ij} = \frac{1}{2V} \int_S (n_i u_j + n_j u_i) \, dA. 
\]  

(20)

Then the average strain in inclusion and matrix is:

\[
\bar{\varepsilon}_{ij}^1 = \frac{1}{2V_1} \int_S (n_i u_j^1 + n_j u_i^1) \, dA = \frac{E_m (3 \kappa_2 + 4 \mu_2)}{3 \kappa_1 + 2 (2 + \kappa_2) \mu_2} \delta_{ij},
\]  

(21a)

\[
\bar{\varepsilon}_{ij}^2 = \frac{1}{2V_2} \int_S (n_i u_j^2 + n_j u_i^2) \, dA = E_m \delta_{ij},
\]  

(21b)

where

\[
\kappa_2 = \frac{\kappa_0}{a \mu}, \quad \mu_s = \frac{\mu_0}{a \mu}, \quad \kappa_0 = 2(\mu_0 + \lambda_0), \quad \eta_0 = 3 \xi_0 + 5 \chi_0, \quad \eta_s = \frac{\eta_0}{a^3 \mu}. \quad (22a-f)
\]

Therefore, the macro strain and stress of the whole RVE can be written as:

\[
E_{ij} = (1 - f) \bar{\varepsilon}_{ij}^2 + f \bar{\varepsilon}_{ij}^1, \quad (23a)
\]

\[
\Sigma_{ij} = f (\bar{\sigma}_{ij}^1 + \tau_{ij}) + (1 - f) \bar{\sigma}_{ij}^2 = 3 \kappa E_{ij}, \quad (23b)
\]

where

\[
\bar{\tau}_{ij} = \frac{1}{V_1} \int_S [\sigma_{ij} n_k x_j] \, dA = \frac{6E_m \kappa_2 \mu_2 (3 \kappa_2 + 4 \mu_2)}{9 \kappa_1 + 6 (2 + \kappa_s) \mu_2} \delta_{ij}. \quad (24)
\]

Substitute the formula (23a) and (24) into (23 b) to solve the equivalent bulk modulus of RVE containing inclusions:

\[
\kappa = \frac{-3 \kappa_1 (3 \kappa_2 + 4 f \mu_2) - 2 \mu_2 (2 \kappa_2 - 6 - 6 f + 3 \kappa_s) + 4 f \kappa_2 \mu_2)}{9 (-1 + f) \kappa_1 - 6 (2 + \kappa_s) \mu_2 + f (-9 \kappa_2 + 6 \kappa_2 \mu_2)} \quad (25)
\]

Considering the inclusion degenerate into holes(\(\kappa_1 = 0\)), the equivalent bulk modulus of nanoporous materials can be simplified as:

\[
\kappa = \frac{-2 \mu_2 (6 - 6 f + 3 \kappa_s) + 4 f \kappa_2 \mu_2}{-6 (2 + \kappa_s) \mu_2 + f (-9 \kappa_2 + 6 \kappa_2 \mu_2)} \quad (26)
\]

### 2.3 Calculation of equivalent shear modulus of the RVE

This subsection aims to solve the equivalent shear modulus of RVE with spherical inclusions or holes. It is assumed that the outer boundary of RVE is subject to the following macroscopic strain of axisymmetric pure eccentric load:

\[
E = \begin{bmatrix} E_e & 0 & 0 \\ 0 & E_e & 0 \\ 0 & 0 & -2E_e \end{bmatrix}. 
\]  

(27)

According to the elastic theory, the displacement field in the inclusion and matrix can be set as:

\[
u_{ij}^1 = \begin{pmatrix} F_{11} R^2 a^2 + F_{12} + F_{13} a^3 \frac{R^3}{R^2} + F_{14} a^5 \frac{R^5}{R^8} \end{pmatrix} R P_2 (\cos \varphi), \quad (28a)
\]

\[
u_{ij}^2 = \begin{pmatrix} G_{11} R^2 a^2 + G_{12} + G_{13} a^3 \frac{R^3}{R^2} + G_{14} a^5 \frac{R^5}{R^8} \end{pmatrix} R \varphi \partial_\varphi P_2 (\cos \varphi), \quad (28b)
\]

\[
u_{ij}^3 = \begin{pmatrix} F_{21} R^2 a^2 + F_{22} + F_{23} a^3 \frac{R^3}{R^2} + F_{24} a^5 \frac{R^5}{R^8} \end{pmatrix} R P_2 (\cos \varphi), \quad (28c)
\]

\[
u_{ij}^4 = \begin{pmatrix} G_{21} R^2 a^2 + G_{22} + G_{23} a^3 \frac{R^3}{R^2} + G_{24} a^5 \frac{R^5}{R^8} \end{pmatrix} R \varphi \partial_\varphi P_2 (\cos \varphi), \quad (28d)
\]

\[
u_{ij}^5 = 0, \quad \nu_{ij}^6 = 0, \quad (28e,f)
\]
where \( P_2 (\cos \phi) \) is a second-order Legendre polynomial with \( \cos \phi \) as the parameter. The strain field can be obtained by substituting the set displacement into the geometric relationship \((13)\), and then the stress field can be obtained by substituting the general Hooke’s law \((14)\). Then the stress can be substituted into the equilibrium equation:

\[
\sigma_{ij} = 0, \quad \sigma_{ij}^2 = 0, \quad (29a,b)
\]

It can be determined that the displacement site contains eight unknown coefficients

\[
G_{11} = \frac{5F_1 \lambda_1 + 7F_1 \mu_1}{6\lambda_1}, \quad G_{12} = \frac{F_1}{2}, \quad (30a,b)
\]

\[
G_{13} = \frac{F_3 \mu_1}{3\lambda_1 + 5\mu_1}, \quad G_{14} = -\frac{F_4}{3}, \quad (30c,d)
\]

\[
G_{21} = \frac{5F_2 \lambda_2 + 7F_2 \mu_2}{6\lambda_2}, \quad G_{22} = \frac{F_2}{2}, \quad (30e,f)
\]

\[
G_{23} = \frac{F_3 \mu_2}{3\lambda_2 + 5\mu_2}, \quad G_{24} = -\frac{F_4}{3}, \quad (30g,h)
\]

Boundary conditions must determine the remaining eight unknown coefficients in the displacement field. First of all, the displacement boundary condition of the outer boundary of RVE with inclusions requires:

\[
u_R^2 \bigr|_{R=b} = 2E_v b. \quad (31)
\]

Two coefficients can be determined by substituting the radial displacement of the matrix into the above formula:

\[
F_{21} = 0, \quad F_{22} = 2E_v. \quad (32a,b)
\]

Secondly, the displacement of the inclusion center should not be singular, which requires:

\[
F_{14} = 0, \quad F_{13} = 0. \quad (33a,b)
\]

Then, the displacement in the matrix and inclusion shall meet the continuity condition at the interface between them:

\[
u_R^2 \bigr|_{R=a} = \nu_R^2 \bigr|_{R=a}, \quad \nu_\phi^2 \bigr|_{R=a} = \nu_\phi^2 \bigr|_{R=a}. \quad (34a,b)
\]

Substitute the radial displacement and polar displacement of matrix and inclusion into the above formula, and use \( F_{12} \) and \( F_{24} \) to represent \( F_{11} \) and \( F_{23} \):

\[
F_{12} = -\frac{7(\lambda_1 + \mu_1)}{5\lambda_1} F_{11} + \frac{2}{5} \left( 1 + \frac{3\mu_2}{3\lambda_2 + 5\mu_2} \right) F_{23} + 2E_v, \quad (35a)
\]

\[
F_{24} = -\frac{(2\lambda_1 + 7\mu_1)}{5\lambda_1} F_{11} - \frac{9(\lambda_2 + \mu_2)}{5(3\lambda_2 + 5\mu_2)} F_{23}. \quad (35b)
\]

Finally, the radial stress and polar stress of inclusion and matrix are substituted into the surface stress boundary condition of Steigmann-Ogden model:

\[
[\sigma]_{ij} n_i = \tau_{ij} + T_{ii} \left( M_{ij,k} n_j \right) - \frac{2}{d} M_{ijkl} m_j n_i, \quad (36)
\]

The \( F_{11} \) and \( F_{23} \) can be gotten.

After obtaining 16 coefficients in the displacement field of inclusion and matrix, the displacement, strain, and stress of RVE-containing inclusion can be completely determined. Next, according to the definition of average strain \((20)\), the average strain of inclusion and matrix can be obtained:

\[
\bar{\varepsilon}_{ij} = -E_b e_x e_x - E_b e_y e_y + 2E_b e_x e_y, \quad (37a)
\]

\[
\bar{\varepsilon}_{ij}^2 = -E_b e_x e_x - E_b e_y e_y + 2E_b e_x e_y, \quad (37b)
\]

where

\[
E_b = \frac{5F_{12} \lambda_1 + 7F_{11} (\lambda_1 + \mu_1)}{10\lambda_1}. \quad (38)
\]
After the average strain in the inclusion and matrix is obtained, the macro strain of the whole RVE containing inclusion can be further determined:

\[ E_{ij} = (1 - f) \varepsilon_{ij}^1 + f \varepsilon_{ij}^2. \]  

(39)

Then the macro stress of the whole RVE can be determined according to the average body stress and the average surface stress:

\[ \Sigma_{ij} = f (\bar{\sigma}_{ij}^1 + \tau_{ij}) + (1 - f) \bar{\sigma}_{ij}^2. \]  

(40)

It can be seen from the macroscopic stress and macroscopic strain constitutive relationship under pure eccentric load condition:

\[ \Sigma_{ij} = 2\mu E_{ij}. \]  

(41)

The equivalent shear modulus of RVE with hole (\( k_1 = \mu_1 = 0 \)) can be calculated from the above formula when the dimensionless coefficient \( m_2 = k_3/\mu_2 \).

\[ \bar{\mu} = \frac{l_1 + l_2 + l_3}{l_4 + l_5 + l_6} \mu_2, \]  

(42)

where

\[ l_1 = f (8 + 9m_2) (-4 - 10\eta_k - 6\eta_s^2 + k_s (-2 + 2\mu_s + \eta_s) + 4\mu_s (1 + 3\eta_s)), \]  

(43a)

\[ l_2 = 2 (16 + 16\eta_k - 36\eta_s^2 + 6k_s (2 + 2\mu_s + \eta_s) + 3m_2 k_s (4 + 2\mu_s + \eta_s)), \]  

(43b)

\[ l_3 = 2 (9m_2 (2 + 2\mu_s - \eta_s) (1 + 2\eta_s) + 8\mu_s (4 + 9\eta_s)), \]  

(43c)

\[ l_4 = 6m_2 (k_s (4 + 2\mu_s + \eta_s) + 3 (2 + 2\mu_s - \eta_s) (1 + 2\eta_s)), \]  

(43d)

\[ l_5 = -6f (2 + m_2) (-4 - 10\eta_k - 6\eta_s^2 + k_s (-2 + 2\mu_s + \eta_s) + 4\mu_s (1 + 3\eta_s)), \]  

(43e)

\[ l_6 = 4 (8 + 8\eta_k - 18\eta_s^2 + 3k_s (2 + 2\mu_s + \eta_s) + 4\mu_s (4 + 9\eta_s)). \]  

(43f)

### 3 Results and discussion

Based on theoretical derivation, this section will quantitatively analyze the effects of surface elastic parameters, surface bending moduli, porosity, and hole radius on nanoporous materials’ macroscopic bulk modulus and shear modulus. For the microscopic RVE, the matrix material is treated as aluminum with the shear modulus \( \mu_2 = 23.6 \) GPa and the bulk modulus \( k = 51.1 \) GPa. Following Duan et al., two sets of surface bulk modulus and shear modulus are considered for nanovoids surface: Case 1 (\( k_0 = 12.932 \) N/Nm, \( \mu_0 = -0.3755 \) N/Nm) and Case 2 (\( k_0 = -5.457 \) N/Nm, \( \mu_0 = -6.2178 \) N/Nm). Three surface parameters are considered for the surface bending moduli of nanovoids, which are additionally considered in the Steigmann–Ogden surface model (\( \eta_0 = 0.30nN \cdot nm \)). The classical solutions without considering the surface effects are listed in the figure as much as possible for comparison.

Fig. 2 shows the curve of normalized equivalent bulk modulus versus hole radius of nanoporous aluminum, where \( k_s \) denotes the classical bulk modulus of porous aluminum. Two sets of surface bulk and shear moduli are considered: case 1 (\( k_0 = 12.932 \) N/Nm, \( \mu_0 = -0.3755 \) N/Nm) and case 2 (\( k_0 = -5.457 \) N/Nm, \( \mu_0 = -6.2178 \) N/Nm). It can be observed that Case 1 effectively increases the equivalent bulk modulus of the nanoporous aluminum, while Case 2 reduces the equivalent bulk modulus. When the size of the hole radius is larger, the surface effect is less noticeable, and the equivalent bulk modulus will be the classical value. In addition, when the porosity is higher, the effect of the surface effect on the control of equivalent bulk modulus will be more obvious.

Fig. 3 depicts the curve of normalized equivalent bulk modulus versus hole radius of nanoporous aluminum, where \( k_s \) denotes the classical bulk modulus of porous aluminum. Two sets of surface bulk and shear moduli are considered: case 1 (\( k_0 = 12.932 \) N/Nm, \( \mu_0 = -0.3755 \) N/Nm) and case 2 (\( k_0 = -5.457 \) N/Nm, \( \mu_0 = -6.2178 \) N/Nm). A phenomenon worth noting is that The surface effect of case 1 can increase the equivalent shear modulus, while case 2 can reduce the equivalent shear modulus. The effect of case 2 on the equivalent shear modulus is much more significant than that of case 1. In addition, when the hole radius is greater than 10 nm, the surface effect will tend to be zero.

Since the formula (26) can find that the equivalent bulk modulus is independent of the surface bending modulus, only the influence of the surface bending modulus on the equivalent shear modulus is explored. Fig. 4 shows the normalized equivalent shear modulus curve versus the hole radius of nanoporous aluminum with different surface bending moduli. Two sets of surface bulk and shear moduli are considered. When the hole radius is greater than 10 nm, the effect of the surface effect on the equivalent bulk modulus will tend to be stable. It is worth noting that the surface bending modulus substantially reduces the equivalent shear modulus of nanoporous aluminum with case 1 crystalline phase but has little effect on case 2.
Figure 2. The curve of normalized equivalent bulk modulus versus hole radius of nanoporous aluminum. Two sets of surface bulk and shear moduli are considered: case 1 ($\kappa_0 = 12.932$ nN/nm, $\mu_0 = -0.3755$ nN/nm, $\eta_0 = 0$) and case 2 ($\kappa_0 = -5.457$ nN/nm, $\mu_0 = -6.2178$ nN/nm, $\eta_0 = 0$).

Figure 3. The curve of normalized equivalent shear modulus versus hole radius of nanoporous aluminum. Two sets of surface bulk and shear moduli are considered: case 1 ($\kappa_0 = 12.932$ nN/nm, $\mu_0 = -0.3755$ nN/nm, $\eta_0 = 0$) and case 2 ($\kappa_0 = -5.457$ nN/nm, $\mu_0 = -6.2178$ nN/nm, $\eta_0 = 0$).
Classical case: \( \eta = 0 \)

\[
\begin{align*}
\text{case 1} & : \eta = 0 \\
\text{case 1} & : \eta = 30 \text{ nN} \cdot \text{nm} \\
\text{case 2} & : \eta = 0 \\
\text{case 2} & : \eta = 30 \text{ nN} \cdot \text{nm}
\end{align*}
\]

Figure 4. The curve of normalized equivalent shear modulus versus hole radius of nanoporous aluminum with different surface bending moduli, where the porosity \( f = 0.2 \). Two sets of surface bulk and shear moduli are considered: case 1 \((\kappa_0 = 12.932 \text{ nN/nm}, \mu_0 = -0.3755 \text{ nN/nm})\) and case 2 \((\kappa_0 = -5.457 \text{ nN/nm}, \mu_0 = -6.2178 \text{ nN/nm})\).

Classical case: \( a = 5 \text{ nm} \)

\[
\begin{align*}
\text{case 1} & : a = 5 \text{ nm} \\
\text{case 1} & : a = 10 \text{ nm} \\
\text{case 2} & : a = 5 \text{ nm} \\
\text{case 2} & : a = 10 \text{ nm}
\end{align*}
\]

Figure 5. The curve of normalized equivalent bulk modulus versus porosity of nanoporous aluminum with different hole radius, where the surface bending modulus \( \eta_0 = 30 \text{nN-nm} \). Two sets of surface bulk and shear moduli are considered: case 1 \((\kappa_0 = 12.932 \text{ nN/nm}, \mu_0 = -0.3755 \text{ nN/nm})\) and case 2 \((\kappa_0 = -5.457 \text{ nN/nm}, \mu_0 = -6.2178 \text{ nN/nm})\).
Fig. 5 draws a curve of normalized equivalent bulk modulus versus porosity of nanoporous aluminum with different hole radius, where the surface bending modulus $\eta_0 = 30\text{nN}\cdot\text{nm}$. It can be seen from the figure that the surface effect will increase the equivalent bulk modulus of case1 crystalline nanoporous aluminum but will reduce the equivalent bulk modulus of case2. When the porosity increases, the influence of the surface effect is more significant. In addition, smaller nanopores have more potent surface effects.

![Figure 5: Curve of normalized equivalent bulk modulus versus porosity](image)

**Figure 6.** The curve of normalized equivalent shear modulus versus porosity of nanoporous aluminum with different hole radius, where the surface bending modulus $\eta_0 = 30\text{nN}\cdot\text{nm}$. Two sets of surface bulk and shear moduli are considered: case 1 ($\kappa_0 = 12.932\ \text{nN}/\text{nm}, \mu_0 = -0.3755\ \text{nN}/\text{nm}$) and case 2 ($\kappa_0 = -5.457\ \text{nN}/\text{nm}, \mu_0 = -6.2178\ \text{nN}/\text{nm}$).

Fig. 6 shows the curve of normalized equivalent shear modulus versus porosity of nanoporous aluminum with different hole radii, where the surface bending modulus $\eta_0 = 30\text{nN}\cdot\text{nm}$. The surface effect will sharply reduce the equivalent shear modulus of case2 crystalline nanoporous aluminum but only slightly increase the equivalent shear modulus of case1 crystalline nanoporous aluminum. In addition, with the increase of porosity, the surface effect will be significantly improved. In addition, the smaller the hole radius, the more significant the surface effect.

4 Concluding remarks

In this paper, we simplified the stress boundary equation of the Steigmann-Ogden surface model. We solved the equivalent bulk modulus and equivalent shear modulus of nanoporous materials based on the homogenization approach. The RVE is described as the classic Mori-Tanaka model, an infinite matrix containing a tiny nanovoid. The surface effects of nanovoids are applied at the interface between the nanovoid and the matrix. Firstly, the stress boundary equation of the Steigmann-Ogden surface model in spherical coordinates is simplified using the index notation method, thus eliminating the influence of the surface gradient operator. Secondly, based on elastic theory, the displacement field is decomposed into static water level displacement and partial displacement fields, which correspond to the solution of equivalent bulk modulus and shear modulus, respectively. And the microscopic uniform modulus. Finally, the homogenization approach obtains the equivalent bulk modulus and shear modulus of nanoporous materials. Based on the theoretical results, many numerical tests were carried out to explore the effects of surface elastic modulus, surface bending modulus, porosity, and hole radius on the equivalent elastic modulus. A few significant conclusions can be drawn based on extensive parametric studies.

- The surface effect is closely related to the hole radius. The smaller the hole radius is, the more pronounced the surface effect is. When the hole radius is greater than 10 nm, the effect of the surface effect will tend to be weak.
- There is a strong positive correlation between surface effect and porosity. The larger the porosity, the more pronounced the surface effect.
- The surface bending modulus does not affect the equivalent shear modulus of nanoporous materials but will reduce the equivalent bending modulus.
- Nanoporous materials with different crystalline phases will have different surface effects.
Acknowledgements

This work was supported by the Innovation Project of Huadong Engineering Corporation Limited [grant numbers KY2023-SD-02-02]

Data Availability

The datasets used and analysed during the current study available from the corresponding author on reasonable request.

References


