

Effective elastic properties of nanoporous materials with hierarchical structure

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Abstract

We investigate the effective elastic properties of nanoporous materials with hierarchical structures, which exhibit a distinct dependence on the characteristic sizes of their microstructure. A core–shell model is first used to account for the effects of both surface tension and surface elasticity. We derive the effective Young's modulus of porous materials with one level of nanosized open or closed cells with surface effects. Then hierarchically structured nanoporous materials consisting of nanosized cells nested in another level of microscaled lattice structure are considered to correlate their effective properties with the hierarchical structure. Particular attention is paid to nanoporous gold with multimodal ligament size distributions.

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1. Introduction

Hierarchical structures spanning the macro, meso, micro to nanoscales are widely observed in many natural materials like wood, cortical bone, deer antler, and glass sponges [1–4]. Having adapted to their living environment through natural evolution over many millions of years, the elegant hierarchical structures endow these biological materials with unusual properties to fulfill their biological functions [5–7]. Inspired by nature, increasing attention has been attracted to the synthesis of artificial porous nanomaterials with hierarchical structures [8–15]. Owing to their huge surface area, controllable pore size and attractive physical properties, nanoporous materials with hierarchical structures hold promise for many technologically important applications in sensing, actuation, catalysis, filtration, and medical engineering [9–18]. For these applications exact characterization of the mechanical behavior of hierarchi-

cally structured nanoporous materials is of great interest. As early as 1993, based on Gibson's scaling law, Lakes established a theoretical model to analyze the stiffness of hierarchical cellular solids [7,19,20]. Recently the elastic properties of nanomaterials with hierarchical and fractal-like topologies have been investigated theoretically [21–23]. Most of these previous models proceeded from the conventional theory of elasticity and predicted that the effective modulus of the materials is size independent. However, recent experiments have shown that such mechanical properties as the elastic modulus and yield strength of nanoporous materials exhibit a distinct dependence on the characteristic sizes of their microstructure [24–27]. How the mechanical properties of nanoporous materials depend on the microstructural sizes however remains elusive.

As is well known, near surface atoms of a material reside in a local environment different from that in the interior and, hence, the surface layer, typically with a thickness of ~ 1 nm, has different mechanical properties and an energy density than its bulk counterpart [28,29]. In hierarchically

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structured nanoporous materials the walls and ligaments of cells can be traced level by level down to the nanoscale, and thus the ratio of surface area to volume increases dramatically. Therefore it is expected that the properties of nanoporous materials are closely related to surface effects. Recently the surface elasticity theory accounting for surface effects has been widely employed to investigate various size-dependent elastic properties of nanosized components [30–32], with good agreement with direct atomic simulations and explain many experimental phenomena [33–39]. Using the theory of surface elasticity, Feng et al. addressed the surface effects on the effective elastic properties of open cell nanoporous materials [40]. To date, however, there is still a lack of investigations on the elastic behavior of nanoporous materials with hierarchical architectures.

In the present paper we theoretically investigate the effective elastic properties of hierarchically structured nanoporous materials using a unit cell model with surface effects. One level nanoporous materials consisting of open or closed cells are first considered to illustrate the effects of residual surface stress and surface elasticity. Then nanoporous materials with two level hierarchical structures are analyzed.

2. One level nanoporous materials

2.1. Gibson's scaling law for porous materials

Based on Gibson's scaling law and the classical continuum theory, Lakes derived the stiffness of hierarchical cellular solids [8,19,20]. The effective elastic modulus was estimated by

$$E_n/E_0 = C^n(\rho_n/\rho_0)^r \quad (1)$$

Here n stands for the hierarchical order number of the material, e.g. $n=0$ corresponds to a continuum and $n=1$ a material with a one level porous structure, E_0 is the Young's modulus of the bulk material ($n=0$), ρ_n and ρ_0 are the mass densities of the foam and the bulk phase, respectively, and C and r are microstructure-dependent constants. For instance, $C=1$ and $r=2$ for open cell foams [19,20]. This model has been widely applied to determine the elastic modulus of foam materials with various hierarchical structures.

2.2. Theory of surface elasticity

In this study the theory of surface elasticity proposed by Gurtin and Murdoch [30] is used to predict the effective elastic properties of hierarchically structured nanoporous materials. We here assume that both the surface layer and the bulk material are isotropic and linearly elastic. Then the constitutive elastic relation of the surface layer is expressed as [33,37]

$$\tau_{\alpha\beta} = \tau_{\alpha\beta}^0 + S_{\alpha\beta\gamma\delta}\varepsilon_{\gamma\delta} \quad (2)$$

where $\tau_{\alpha\beta}$ is the surface stress tensor, $\varepsilon_{\gamma\delta}$ the surface strain tensor, $S_{\alpha\beta\gamma\delta}$ the surface stiffness tensor, and $\tau_{\alpha\beta}^0$ the residual

surface stress when the bulk is unstrained. Most surfaces, especially those in crystalline materials, have anisotropic properties, and they can induce large and systematically anisotropic strain in the bulk of nanoporous materials, as described by Weissmüller et al. [41,42]. For the sake of simplicity, however, we assume that the surfaces in the nanoporous material considered is isotropic, or, in others words, they have orientation-averaged elastic properties. In this case the constitutive relation in Eq. (2) reads [30,31]

$$\tau_{\alpha\beta} = \tau_{\alpha\beta}^0 + 2\mu_s\varepsilon_{\alpha\beta} + \lambda_s\varepsilon_{\gamma\gamma}\delta_{\alpha\beta} \quad (3)$$

where λ_s and μ_s are the surface Lamé constants and $\delta_{\alpha\beta}$ is the Kronecker delta. The constitutive relation in Eq. (3) can also be written in other forms [43]. When the surface is subjected to uniaxial tension Eq. (3) can be further simplified as [33,37]

$$\tau = \tau^0 + E_s\varepsilon \quad (4)$$

where τ is the surface stress, ε is the surface strain, and τ^0 the residual surface stress under unstrained condition [37]. The parameter E_s is referred to as the surface Young's modulus, which was initially defined by Gurtin and Murdoch [30]. It is related to the surface Lamé constants via $E_s = 2\mu_s + \lambda_s$. Theoretically the value of E_s may be positive or negative, depending on the crystalline structure and the orientation of the surface [32,38]. For different materials, therefore, the elastic modulus of a nanowire may either increase or decrease with decreasing size.

2.3. Open cell nanoporous materials

Analogously to the classical Gibson–Ashby theory [19,20], an open cell nanoporous material is modeled as a three-dimensional network consisting of a periodically and infinitely extending array of identical unit cells. We choose a cubic unit cell containing 24 ligaments, as shown in Fig. 1a. Unit cells of other types can be analyzed similarly.

For nanoporous materials the characteristic size of these ligaments reduces to nanometers. Both elaborate experiments and atomic simulations have demonstrated that surface effects may have a remarkable influence on the mechanical behavior of such nanosized structural elements as nanobeams, nanowires, and nanoparticles [33–39]. In the present paper we employ the core–shell model to examine the surface effects in nanoporous materials, and introduce a thin surface layer with uniform thickness t_0 and Young's modulus E_t covering all surfaces of the ligaments. To regenerate the idealized surface with zero thickness assumed in the surface elasticity theory we let t_0 approach 0 while $E_t t_0$ is kept as the constant of surface stiffness E_s , i.e. $E_t t_0 = E_s$.

To calculate the effective Young's modulus of the porous material a macroscopic uniform tensile stress σ_1 is assumed along the Z direction. Here and in the following we use the subscripts 1 and 2 to indicate the parameters of a porous material with one and two level structure,

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