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Finite element characterization of the size-dependent mechanical behaviour in nanosystems

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Abstract
Mechanical behaviour analysis plays an important role in the design of micro/nano-electromechanical system (MEMS/NEMS) devices for reliability. In this paper, the size-dependent mechanical properties of nanostructures are numerically studied with the finite element method (FEM) by developing a kind of surface element to take into account the surface elastic effect. This method is then applied to the investigation of the interaction between two pressurized nanovoids and the effective moduli of two-dimensional nanoporous material. The numerical results indicate that surface elasticity can significantly alter the nature of interaction forms and the effective moduli by inducing a strong size dependence in conventional results.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The advent of nanotechnology has facilitated the fabrication of many nanosystems such as nanoelectromechanical systems (NEMS) and nanocomposites. As compared with their bulky counterparts, they possess many superior performances, e.g. better mechanical or electric properties. However, due to the high ratio of the surface area to the volume of the bulk, the properties of the nanosystems exhibit size dependent behaviour. Such phenomena have been observed in many mechanical experiments on nanobeams [1] and carbon nanotubes [2, 3]. Meanwhile, much theoretical research has been done on such subjects. For instance, a generic continuum model incorporating surface effects was first elaborated by Gurtin and Murdoch [4] through introducing surface elasticity into the conventional theory of elasticity. Based on this theory, Miller and Shenoy [5] studied the size-dependent elastic behaviour of some basic nanostructural elements such as nanobars and nanoplates under tension and pure bending; Sharma *et al* [6, 7] and Duan *et al* [8] provided closed-form expressions for the size-dependent elastic state of nanosized inhomogeneities; the latter authors [9] also theoretically predicted the size dependence of the effective modulus of a composite containing spherical inhomogeneities at nanometre length scale; Dingreville *et al* [10] analysed the size-dependent effective moduli of isolated nanosized elements (particles, wires and films); He *et al* [11] provided a continuum model for size-dependent deformation of nano films. All these analyses came to the same conclusion that surface elasticity plays an important role in the mechanical response of systems in the nanometre range.

It should be noted that the above-mentioned theoretical works are confined to systems of simple geometry, and the analytical solutions are far more difficult for systems with slightly more complex geometry. It is reported by Gilbert *et al* [12] that nanoparticles appear with irregular surfaces when their radii are in the range of about 3 nm. Therefore, to further elucidate the surface elastic effect and better characterize mechanical behaviour of nanosystems, numerical methods such as the finite element method (FEM) should be a good alternative. However, the traditional FEM can only provide size-independent numerical solutions due to the failure in capturing the surface effect. With this in mind we present a new finite element formulation in this work by incorporating the surface elasticity with the conventional one. Based on the new formulation, two examples are further studied, i.e., the

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interaction between pressurized nanovoids and the effective moduli of nanoporous materials.

2. Basic theory of surface elasticity

Continuum theories taking into account the surface effects have been developed by several authors [4–11]. In this section, we only present the essentials of such theories. Under a reasonable assumption, the surface can be regarded as a negligibly thin object adhering to the underlying material without slipping. First, the surface should satisfy the equilibrium equation [5]:

$$\begin{aligned} \sigma^{\mathrm{s}}_{\alpha\beta,\beta} + t_\alpha &= 0, \\ \sigma^{\mathrm{s}}_{\alpha\beta}\kappa_{\alpha\beta} = \sigma^{\mathrm{b}}_{ij} n_i n_j \qquad & (i,j=1,2,3 \quad \alpha,\beta=1,2) \end{aligned} \tag{1}$$

where $\sigma^{\mathrm{s}}_{\alpha\beta}, \sigma^{\mathrm{b}}_{\alpha\beta}$ are the surface stress and bulk stress respectively, n_i the normal to the surface, t_α the component of the traction $\sigma^{\mathrm{b}}_{ij} n_j$ along the α direction along the surface and $\kappa_{\alpha\beta}$ the curvature tensor.

According to [13], the surface stress $\sigma^{\mathrm{s}}_{\alpha\beta}$ is related to the deformation dependent surface energy γ by Shuttleworth's equation:

$$\sigma^{\mathrm{s}}_{\alpha\beta} = \gamma\delta_{\alpha\beta} + \frac{\partial\gamma}{\partial\varepsilon^{\mathrm{s}}_{\alpha\beta}} \tag{2}$$

where $\varepsilon^{\mathrm{s}}_{\alpha\beta}$ is the surface strain tensor. As given in [5], a linear constitutive relationship between surface stress and surface strain can be written:

$$\sigma^{\mathrm{s}}_{\beta\alpha} = \tau^0_{\alpha\beta} + S_{\alpha\beta\gamma\delta}\varepsilon^{\mathrm{s}}_{\gamma\delta} \tag{3}$$

where $S_{\alpha\beta\gamma\delta}$ is the elastic constants for the surface and can be determined from atomistic calculations and $\tau^0_{\alpha\beta}$ the residual surface stress when the bulk is unstrained.

3. Finite element formulation for surface elasticity

The total potential energy Π consists of three parts: the bulk elastic energy U^{b}, the work of external force W, and surface elastic energy U^{s}, that is

$$\Pi = U^{\mathrm{b}} + U^{\mathrm{s}} - W \tag{4}$$

where U^{b} and W can be calculated in bulk elements as in classical theory, while U^{s} must be calculated through the surface element, which can be expressed as

$$\begin{aligned} U^{\mathrm{s}} &= \int\int_\Omega \{\sigma^{\mathrm{s}}\}^{\mathrm{T}}\,\mathrm{d}\{\varepsilon^{\mathrm{s}}\} \\ &= \int\int_\Omega ([S]\{\varepsilon^{\mathrm{s}}\} + \{F\})^{\mathrm{T}}\,\mathrm{d}\{\varepsilon^{\mathrm{s}}\} \\ &= \tfrac{1}{2}\int\int_\Omega \{\varepsilon^{\mathrm{s}}\}^{\mathrm{T}}[S]\{\varepsilon^{\mathrm{s}}\}\,\mathrm{d}\Omega + \int\int_\Omega \{\varepsilon^{\mathrm{s}}\}^{\mathrm{T}}\{F\}\,\mathrm{d}\Omega \end{aligned} \tag{5}$$

where Ω represents the domain of the surface element and $[S]$ and $[F]$ are defined as the surface elastic matrix and residual surface stress matrix respectively. The surface strain can be written as $\{\varepsilon^{\mathrm{s}}\} = [B^{\mathrm{s}}]\{\delta_{\mathrm{e}}\}$, where $[B^{\mathrm{s}}]$ is the strain–displacement matrix of the surface element and $\{\delta_{\mathrm{e}}\}$ the displacement matrix of the element node. Substituting this relation into (5) yields

$$U^{\mathrm{s}} = \tfrac{1}{2}\int\int_\Omega \{\delta_{\mathrm{e}}\}^{\mathrm{T}}[K^{\mathrm{s}}_{\mathrm{e}}]\{\delta_{\mathrm{e}}\}\,\mathrm{d}\Omega + \int\int_\Omega \{\delta_{\mathrm{e}}\}^{\mathrm{T}}\{P^{\mathrm{s}}_{\mathrm{e}}\}\,\mathrm{d}\Omega \tag{6}$$

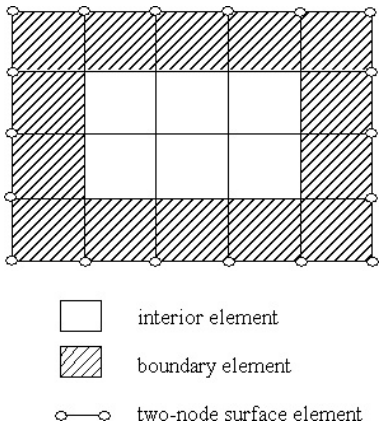

Figure 1. Schematic diagram of mesh map of solid containing surface elements.

with $[K^{\mathrm{s}}_{\mathrm{e}}]$ defined as the surface stiffness matrix,

$$[K^{\mathrm{s}}_{\mathrm{e}}] = \int\int_\Omega [B^{\mathrm{s}}]^{\mathrm{T}}[S][B^{\mathrm{s}}]\,\mathrm{d}\Omega \tag{7}$$

and $[P^{\mathrm{s}}_{\mathrm{e}}]$ as the surface residual stress matrix.

$$\{P^{\mathrm{s}}_{\mathrm{e}}\} = \int\int_\Omega [B^{\mathrm{s}}]^{\mathrm{T}}\{F\}\,\mathrm{d}\Omega. \tag{8}$$

Then equilibrium equations can be obtained from the functional stationary condition $\delta\Pi = 0$, respectively for the interior elements and boundary elements that are shown in figure 1:

$$\begin{aligned} &[K_{\mathrm{e}}]\{\delta_{\mathrm{e}}\} = [P_{\mathrm{e}}], \qquad \text{for interior elements} \\ &\{[K_{\mathrm{e}}] + [K^{\mathrm{s}}_{\mathrm{e}}]\}\{\delta_{\mathrm{e}}\} = [P_{\mathrm{e}}] - [P^{\mathrm{s}}_{\mathrm{e}}], \\ &\qquad \text{for boundary elements} \end{aligned} \tag{9}$$

where $[K_{\mathrm{e}}]$ and $[P_{\mathrm{e}}]$ are respectively the stiffness matrix and nodal force matrix corresponding to the bulk element. From (9) one can see that the effect of surface elasticity is to change the stiffness matrix and nodal force only on the boundary.

With the above principle, one can design surface elements and calculate the corresponding $[B^{\mathrm{s}}]$, $[K^{\mathrm{s}}_{\mathrm{e}}]$ and $[P^{\mathrm{s}}_{\mathrm{e}}]$ for any purpose of use. The present work specifically designs a two-node surface element applicable for plane strain and axisymmetric problems which are studied in the following numerical examples. By virtue of being attached to volume elements, this surface element can reflect the surface stiffness and transmit the residual surface stress to the material.

4. Numerical examples

4.1. Numerical verification of the surface element

To verify the validity of the proposed surface element formulation, a problem of stress concentration at a nanoscaled spherical void under hydrostatic loading is studied here. The corresponding analytical solution has been given by Sharma *et al* [6]. Therein they considered isotropic surfaces and $\tau_0 = 0$. Consequently, the surface constitutive relationship reads

$$\sigma^{\mathrm{s}}_{\beta\alpha} = 2\mu_{\mathrm{s}}\delta_{\beta\gamma}\varepsilon_{\gamma\alpha} + \lambda_{\mathrm{s}}\varepsilon_{\gamma\gamma}\delta_{\beta\alpha} \tag{10}$$

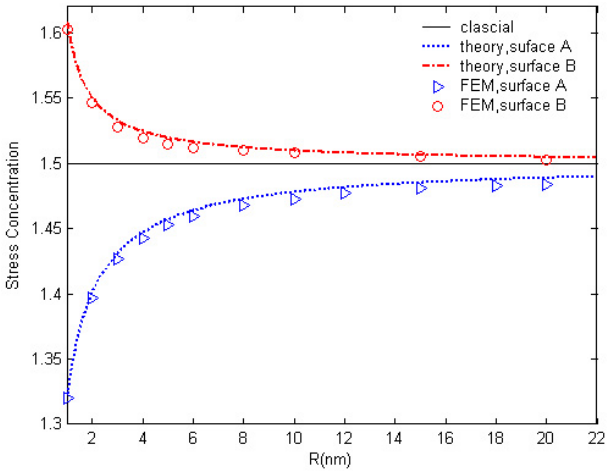

Figure 2. Variation of stress concentration with the void radius R.

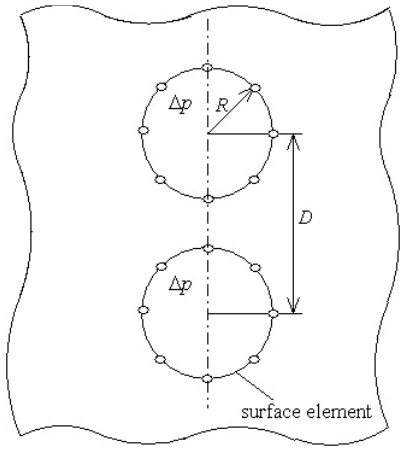

Figure 3. Schematic diagram of two nanovoids attached by surface elements in an infinite domain.

Table 1. Surface elastic constants for Al. Units are N m^{-1}.

Type	Surface	λ_s	μ_s	K_s
A	Al[111]	6.842	−0.3755	12.932
B	Al[100]	3.489	−6.2178	−5.457

in which λ_s and μ_s are surface Lamé constants and a 'surface modulus' can be defined by $K_s = 2(\mu_s + \lambda_s)$. Two types of surface constants are presented for isotropic surfaces [14], namely, surface A and surface B as denoted in table 1, which roughly correspond to respectively the crystal planes [111] and [100] of aluminium as the surfaces. The numerical results from the present FEM and the theoretical results [6] are compared in figure 2. It can be seen from this figure that the numerical results are in good agreement with analytical solutions, which speaks well of the validity of the present surface element. Consequently we can use it with much confidence hereafter.

4.2. The interaction between two nanovoids with surface effects

In this subsection, special attention is placed on the interaction energy between two voids. It plays an important role in the mechanical behaviour of porous materials, for example, the reliability of materials [15, 16]. The interaction problem between voids has been conventionally investigated as bubbles that are formed by helium atoms produced by nuclear fission [17], and the point-defect as centres of dilatation [18]. Unanimously the surface elastic effect has been neglected in all those investigations and may be important when the voids are in the nanometre range. Consider two spherical nanovoids of radius R subject to uniform internal pressure Δp in an infinite domain and separated by a distance D along the line between their centres. To analyse such an interaction problem with surface effects by FEM, the surface elements should be attached on the surface of the voids as illustrated in figure 3, or alternatively the stiffness matrix and nodal forces of the elements at the surface should be calculated according to the second formulae in (9). The material is assumed to be aluminium with Young's modulus $E = 75.3$ GPa and Poisson's ratio $\nu = 0.3$, and two sets of surface elastic constants A and B are taken from table 1. To investigate the effect of surface modulus K_s, the contribution of the residual stress τ_0, just like the internal pressure Δp, is not considered here.

The interaction energy Φ_{int} between two voids can be defined as

$$\Phi_{int} = \Phi_2 - 2\Phi_1 \tag{11}$$

where Φ_1 is the total potential for the infinite system with only one void, and Φ_2 that for the same system with two voids. It can be shown easily that

$$\Phi_1 = U_1 - W_1 = -\tfrac{1}{2}W_1, \qquad \Phi_2 = U_2 - W_2 = -\tfrac{1}{2}W_2 \tag{12}$$

where U_1 and W_1 are respectively the elastic energy including both bulk and surface contributions, and the work done by internal pressure Δp for the one-voided system, while U_2 and W_2 are the counterparts for the two-voided system. Substituting (12) into (11) yields $\Phi_{int} = -\frac{1}{2}W_2 + W_1$, through which the interaction energy can be conveniently obtained.

For brevity, define $\Phi^*_{int} = (\Phi^s_{int} - \Phi^0_{int})/(|\Phi^0_{int}|)$, where Φ^s_{int} (<0) and Φ^0_{int} (<0) respectively represent the interaction energy with surface effects and the classical one without surface effects. Figure 4 displays the variation of Φ^*_{int} for two sets of surface properties as a function of the void radius when $D/R = 2.1$ and $\Delta p = 1$ MPa. It can be seen from figure 4 that for a given ratio of D/R surface elasticity causes Φ^*_{int} to increase with decreasing void size for $K_s > 0$ (the curve denoted by surface A) and to decrease for $K_s < 0$ (the curve denoted by surface B), while the classical result ($K_s = 0$) is independent of the void size. Figure 4 also implies that the voids remain more stable on surface B because of the lower energy in this case.

The variations of Φ_{int} ($R = 2$ nm, $\Delta p = 1$ MPa) as the distance D between the two voids are plotted in figure 5 for three cases, i.e. surface A ($K_s > 0$), surface B ($K_s < 0$) and classical surface ($K_s = 0$). From the figure we can find the interaction energy reduces with decreasing void distance D, which indicates that the two pressurized voids will attract each other. We also note that the curve corresponding to surface B ($K_s < 0$) has the largest slope among the three cases, which indicates that the two voids would attract each

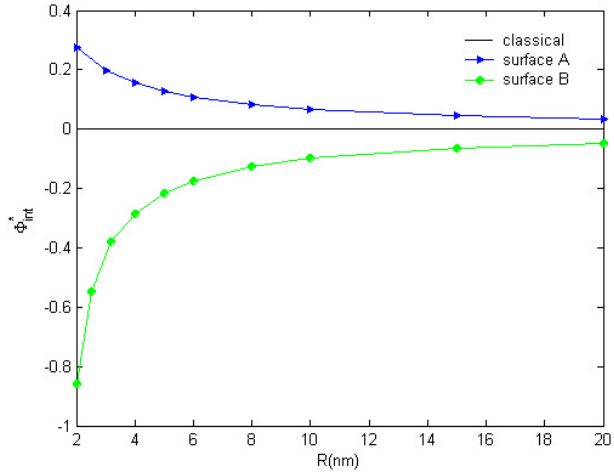

Figure 4. Variation of the value of Φ^*_{int} as the radius of the void.

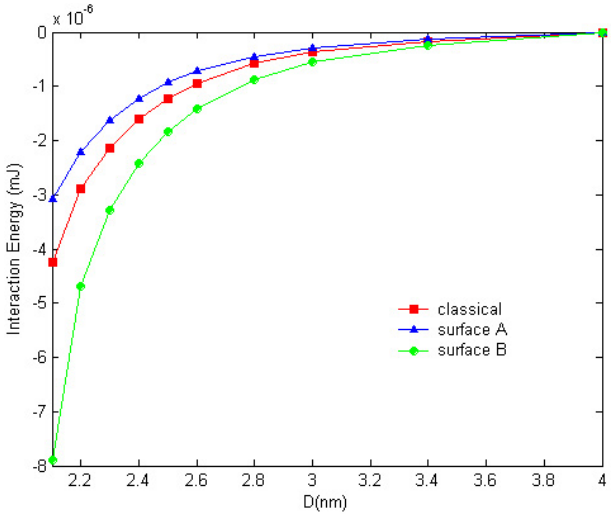

Figure 5. Variation of the interaction energy as the distance between two voids.

other most strongly and diffuse more easily on surface B. The magnitude of Δp can change the absolute value of Φ_{int} but not the relative relationship among the curves corresponding to the three cases. Finally, it is worth pointing out that as mentioned earlier one of the effects of surface elasticity in the case of the present finite element formulation is to alter the stiffness matrix of the elements at the surface, and for negative surface modulus the stiffness matrix may be modified such that the diagonal elements no longer dominate, which would influence the condition number of the total stiffness matrix. In fact, our numerical study (not shown) demonstrates that the larger the absolute value (or the smaller the dimension) is, the larger the condition number of the total stiffness matrix is, which may consequently tend to be ill conditioned, although the total energy (bulk + surface) needs to satisfy the positive definiteness condition as pointed out by Shenoy [19]. Moreover, when the ill condition leads to inaccurate results, special numerical methods should be applied to improve the precision of solutions; however, these methods are not discussed in the present work. For the above example, it is possible to obtain reliable computational results for a void radius R larger than 2 nm.

4.3. Effective properties of two-dimensional solid containing nanovoids

In the mechanical characterization of the nanoporous materials, effective moduli are important parameters. Due to the nanovoids contained in the materials, their effective moduli may exhibit size-dependent behaviour. Taking surface elasticity into consideration, Duan *et al* [9] have obtained analytic results for a composite containing spherical inhomogeneities. As another application of the present surface element, we calculate the effective moduli of two-dimensional nanoporous material. To this end, consider nanovoids are arranged periodically in a solid under the plane strain condition. Due to this assumption, it is possible to identify a two-dimensional unit cell as a representative volume element (RVE) and the surface elements are attached on the surface of the void. See the illustration in figure 6. Then effective bulk modulus that reflects the relationship between

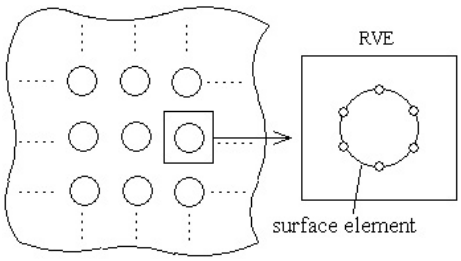

Figure 6. Schematic diagram of periodic arrays of nanoporous solid and RVE.

the mean stress and the variation of area, and the effective Young's modulus, can be directly calculated according to their definition. The details of the calculation process are omitted here for the sake of brevity and can be found in [20].

The bulk and surface properties of the solid are taken as the same as those in section 4.2. We define $K^*_{\text{eff}} = (K^{\text{s}}_{\text{eff}} - K^0_{\text{eff}})/K^0_{\text{eff}}$ and $G^*_{\text{eff}} = (G^{\text{s}}_{\text{eff}} - G^0_{\text{eff}})/G^0_{\text{eff}}$, where $K^{\text{s}}_{\text{eff}}$ and $G^{\text{s}}_{\text{eff}}$, K^0_{eff} and G^0_{eff}, respectively represent the effective bulk modulus and shear modulus with surface effects and the classical ones without surface effects under the plane strain condition. The variations of K^*_{eff} and G^*_{eff} as the void radius are plotted in figures 7 and 8 when the volume fraction $f = 0.3$ (defined as the ratio between the volume of voids and total volume), where we can find that their values represent a deviation from the classical results, and the smaller the nanovoids the larger the deviation. Figures 7 and 8 also demonstrate that the surface effects on the bulk modulus and shear modulus are almost the same. Meanwhile, it is worth highlighting that when subjected to hydrostatic loading and shear loading the surface elasticity can make the nanoporous material stiffer or softer than the classical case without the surface effect, which depends on the surface elastic constants, and this effect will become more pronounced with decreasing void size and increasing volume fraction of voids. Like the case in section 4.2, when the surface stiffness is negative, with

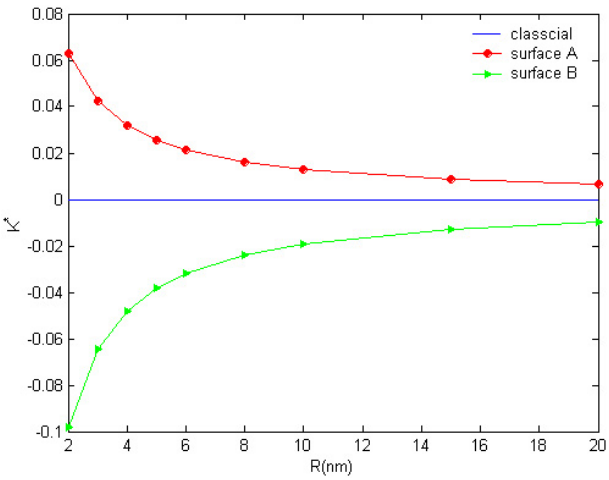

Figure 7. The variation of K^* as the radius of the nanovoid.

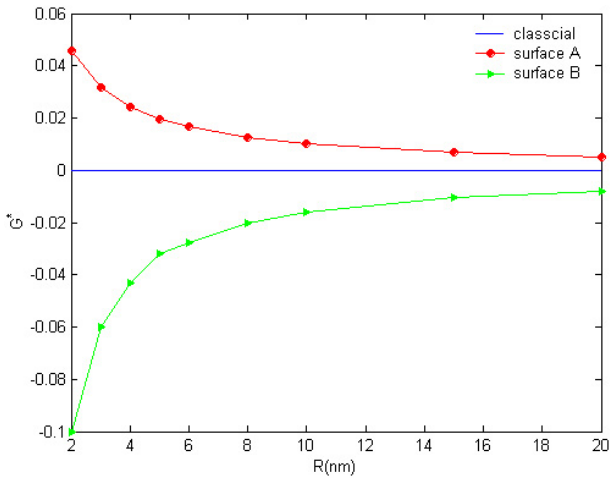

Figure 8. The variation of G^* as the radius of the nanovoid.

the diminution of the structure's dimension, the total stiffness matrix of the problem becomes ill conditioned. However, in this problem the results are reliable enough when void radius R is larger than 2 nm.

5. Concluding remarks

The finite element formulation which accounts for surface elasticity has been derived from the potential energy functional to describe the size dependence of the mechanical properties in nanosystems. Its validity has been verified from the stress concentration at a nanovoid. The newly developed surface element has then been applied to the investigation of surface effects in the interaction between nanovoids and the effective moduli in nanoporous materials. Some valuable mechanical and physical behaviours of nanosystems different from the classical elasticity are studied in detail. Numerical results for the interaction between two nanovoids show that the interaction intensity is enhanced or weakened with decreasing void radius for a given ratio of D/R; the surface effect also has a significant influence on the effective properties of nanoporous materials.

It should be noted that the surface element developed in this paper is reliable and can conveniently facilitate the study of surface elastic effects in many other nanosized problems, for instance the mechanical response of some nanostructural elements such as nanobeams, nanobars, nanoplates etc. Meanwhile, the idea of our derived surface element can be generalized to study the effects of the interface by developing a kind of interface element, if the interface elastic constants are known. Finally, as mentioned above for some problems the large absolute value of negative surface modulus brings about an ill conditioned total stiffness matrix, therefore effective numerical methods to deal with the ill defined problem and improve the precision of solutions are worthwhile to include in future work.

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