On the theory of plates and shells at the nano- and microscales considering surface effects

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Phenomena

- The development of nanotechnologies extends the field of application of the classical or non-classical theories of plates and shells towards the new thin-walled structures.
- In general, modern nanomaterials have physical properties which are different from the bulk material.
- The classical linear elasticity can be extended to the nanoscale by implementation of the theory of elasticity taking into account the surface stresses, cf. Duan et al. (2008) among others.
- In particular, the surface stresses are responsible for the size-effect, that means the material properties of a specimen depend on its size.
- For example, Young’s modulus of a cylindrical specimen increases significantly, when the cylinder diameter becomes very small.
- The surface stresses are the generalization of the scalar surface tension which is well-known phenomenon in the theory of capillarity.
Our Aim is

- to discuss the effective constitutive equations for surface stresses taking into account complex structure of surface and/or surface coatings;
- to analyze of the influence of surface effects on the effective properties of materials such as the effective bending stiffness of plates or the stiffness of rods.

Surface elasticity models

- Based on additional surface (2D) constitutive equations. After Laplace (1805) and Young (1806).
- Based on unified gradient-type models. After van der Waals (1893) and Korteweg (1901).
- With sharp interface or
- with interfacial layer.
Surface Elasticity

- The investigations of the surface phenomena were initiated by Laplace (1805), Young (1806) & Gibbs (1875-1878).
- Works taking into account the surface stresses
  - Gurtin & Murdoch (1975)
  - Podstrigach & Povstenko (1985)
  - Steigmann & Ogden (1999)
- Residual surface stresses
  - Gurtin, Markenscoff, and Thurston (1976);
  - Wang and Feng (2007);
  - Wang and Zhao (2009).
- FEM realization
- Reviews
  - Orowan (1970)
  - Podstrigach & Povstenko (1985)
  - Finn (1986)
  - Rusanov (2005)
  - Duan, Wang & Karihaloo (2008)
  - Wang et al. (2011)
Surface tension
Surface tension may be useful
Influence of Surface Stresses

**Phase transitions**
Nucleation, crystal growth, etc.

**Fracture mechanics**
Griffith criterion, Effective surface energy density, Line tension as a energy of a dislocation core

**Mechanics of porous media**
Nanoporous materials can be made stiffer than non-porous counterparts by surface modification

**Other problems**
Surface diffusion, Surface waves.
Influence of Surface Stresses

**Phase transitions**
Nucleation, crystal growth, etc.

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**Other problems**
Surface diffusion, Surface waves.
Experimental Observations (I)

Surface stresses → size effect

Young’s modulus, experimental data: eigenfrequencies of nanowires

$^a$Chen et al. (2006)
Experimental Observations (II)

Size effect

Young’s modulus: bending of nanobeams made of Ag, Pb\textsuperscript{a,b}

\begin{itemize}
  \item \textsuperscript{a}Cuenot et al. (2004)
  \item \textsuperscript{b}Jing et al. (2006)
\end{itemize}
Experimental Observations (III)

Size effect

Young modulus: bending of nanoplates\textsuperscript{a}
(molecular dynamics estimations)

\textsuperscript{a}Wang et al. (2006)
**Size effect**

Nanoporous materials can be made stiffer\(^a\)

\(^a\)Duan et al. (2005, 2008)
Experimental Observations (V)

Size effect

Dependence of the effective moduli on the size of pores

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Fig. 5.1 Effective bulk modulus as a function of void radius ($f = 0.3$). A: $\kappa_s = -5.457 \text{ N/m}$, $\mu_s = -6.2178 \text{ N/m}$ for the surface [1 0 0]; B: $\kappa_s = 12.932 \text{ N/m}$, $\mu_s = -0.3755 \text{ N/m}$ for the surface [1 1 1]; C: the classical results without the surface stress effect. Reprinted from Duan et al. (2005b)

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$^a$Duan et al. (2005)
Wang et al. (2006), Duan et al. (2008): Dependence on the size length $L$.

Let $F$ be some property, i.e. Young’s modulus, temperature of melting, etc. Then we assume

$$\frac{F(L)}{F(\infty)} = 1 + \alpha \frac{l_{in}}{L} + O\left(\frac{l_{in}}{L}\right)^2$$

Example: temperature of melting of a nanoparticle of radius $R$ are

$$\frac{T(R)}{T(\infty)} = 1 - 2 \frac{l_{in}}{R}$$

Here $l_{in}$ is a characteristic length, usually $l_{in} = 2\ldots20$ nm.
What type of surface may we have?

- Perfect and
- Non-Perfect. Is it really surface?
Perfect surfaces – planes and mathematical surfaces

ZnO crystal, ZnO nanotubes, etc.
Non-Perfect surface

Broadband omnidirectional antireflection coating

Self-cleaning polymer coating

Cross-Linked Polyacrylate Nanofiber Arrays

Elastic Body with Surface Stresses

Reference configuration

\[ t_s = t + \nabla_s \cdot S \]

\[ \Omega = \Omega_s \cup \Omega_u \cup \Omega_f \]

\[ \Omega_s = \Omega_- \cup \Omega_+ \]
Boundary-value Problem

Elastic body with surface stresses\(^1\):

\[
\nabla_x \cdot P + \rho f = 0, \quad (n \cdot P - \nabla_s \cdot S)|_{\Omega_s} = t, \\
u|_{\Omega_u} = 0, \quad n \cdot P|_{\Omega_f} = t.
\]

Here \(P\) is the first Piola-Kirchhoff stress tensor, \(\nabla_x\) the 3D nabla operator, \(\nabla_s\) the surface (2D) nabla operator, \(S\) the surface stress tensor of the first Piola-Kirchhoff type acting on the surfaces \(\Omega_s\), \(u = x - X\) the displacement vector, \(f\) and \(t\) the body force and surface loads vectors, respectively, and \(\rho\) the density.

We assume that the part of body surface \(\Omega_u\) is fixed, while on \(\Omega_f\) the surface stresses are absent.

\(^1\)Gurtin and Murdoch, Arch. Rat. Mech. Analysis, 1975
Basic assumptions

Additional constitutive equation for surface

\[ U = U(F), \quad F = \nabla_s x_s, \quad S = \frac{\partial U}{\partial F}, \]

or more general equations like as for example

\[ U = U(F, \nabla_s F, \ldots). \]

Compatibility

\[ x_s \equiv x \big|_{\Omega_s} \]

or more general like as

\[ x_s \equiv \mathcal{A} \left( x \big|_{\Omega_s} \right) \]
Constitutive Relations

For the bulk material we use the relations

\[ P = \frac{\partial W}{\partial \nabla x}, \]

where \( W \) is the strain energy density.

In the theory of Gurtin & Murdoch (1975) the tensor \( S \) is similar to the membrane stress resultants.

\[ S = \frac{\partial U}{\partial F}, \]

where \( U \) is the surface strain energy density.

**Residual stresses:** In this case we assume that \( W \) and \( P \) possess the properties \( W(I) = 0, \quad P(I) = 0 \), while there exist residual (initial) surface energy and surface stresses that is

\[ U(A) = U_0 \neq 0, \quad S(A) = S_0 \neq 0, \]

where \( I \) and \( A \equiv I - N \otimes N \) are the 3D and surface unit tensors, respectively. Further we consider the influence of \( U_0 \) and \( S_0 \) on the effective ( apparent) properties of solids.
Linearized Relations

In the case of infinitesimal strains of an isotropic body we have the following constitutive equations

\[ P = 2\mu \varepsilon + \lambda \text{tr} \varepsilon, \quad S = S_0 + 2\mu_S \varepsilon + \lambda_S \text{tr} \varepsilon + S_0 \cdot \nabla_s u, \]

where

\[ \varepsilon = \frac{1}{2} \left( \nabla u + (\nabla u)^T \right), \quad \varepsilon = \frac{1}{2} \left( \nabla_S v_s \cdot A + A \cdot (\nabla_S v_s)^T \right), \]

I the 3D unit tensor, \( A \equiv I - n \otimes n, \ v_s = u \bigg|_{\Omega_s} \) .

See restrictions for \( \lambda, \mu \) and \( \lambda_S, \mu_S \) in Altenbach et al. (2010); Javili and Steinmann (2012):

\[ \mu > 0, \quad 3\lambda + 2\mu > 0; \quad \mu_S > 0, \quad \lambda_S + \mu_S > 0. \]

But \( S_0 \) is an arbitrary second-order tensor, in general.
Surface moduli $\lambda^S_{\pm}$, $\mu^S_{\pm}$ can be determined together with the bulk moduli. A possible way is the use of the size effect, i.e. this means the using the experiments for beams with various cross-section diameters.

\[ \text{Cuenot et al. (2004)} \]
Comparison of three-layered plate and plate with surface stresses

For \( h_f \to 0 \) with accuracy up to \( O(h_f^2) \) from comparison of the tangential and bending stiffness parameters is follows that\(^3\)

\[
\mu_S = \lim_{h_f \to 0} \mu_f h_f, \quad \lambda_S = \lim_{h_f \to 0} \lambda_f \frac{1 - 2\nu_f}{1 - \nu_f} h_f.
\]

\(^3\)Altenbach et al. Mechanics of Solids. 2010
Porous rod\textsuperscript{4}

Tension–compression, elementary formula of the strength of materials

\[ E^* = E (1 - \varphi) \]

where \( \varphi = S/F \) is the porosity.

\checkmark No influence of surface effects

\textsuperscript{4}Eremeyev and Morozov, Doklady Physics, 2010
Question: For which cross sections shown in Figure the effective Young’s modulus is higher?

Two cross sections of the rod with the identical porosity (with an identical pore area $S$)
Effective Young’s Moduli. Various Approaches

- Theory of surface stresses

\[ E_S^* = E(1 - \varphi) + E_S \frac{2\sqrt{S}}{\sqrt{\pi F}} \sqrt{n} = E_*^* + E_S \frac{2\sqrt{S}}{\sqrt{\pi F}} \sqrt{n}. \]

- Surface layer (Mechanics of composites)

\[ E_f^* = E \left(1 - \frac{S + S_\delta}{F}\right) + E_f \frac{S_\delta}{F} = E_*^* + (E_f - E) \frac{S_\delta}{F}, \]

where \( S_\delta(n) = \pi n [(r + \delta)^2 - r^2] \) is the area of the surface layers and, finally,

\[ E_f^* = E_*^* + (E_f - E) \frac{2\delta \sqrt{\pi S}}{F} \sqrt{n}. \]

- Complex formula

\[ E^* = E_*^* + E_S \frac{2\sqrt{S}}{\sqrt{\pi F}} \sqrt{n} + (E_f - E) \frac{S_\delta(n)}{F}. \]
Effective Young’s Moduli. Various Approaches

Dependencies of $E^*$, $E^*_o$, $E^*_S$ and $E^*_f$ on $\sqrt{n}$ for $E_f > E$ (on the left) and for $E_f < E$ (on the right)
Effective Young’s Moduli. Various Approaches. II

$E^*$ depends on the values of $h_f$, $R$, $E_S$, and $E$. Here $d = 2E_S/E$ is the characteristic length parameter introduced in Duan et al. (2008), Wang et al. (2006).

Effective Young modulus $E^*$ as the function of radius $R$: a) $E_f > E$, b) $E_f < E$. 

![Graphs showing the variation of effective Young's modulus ($E^*$) with radius ($R$) for different cases: a) $E_f > E$, b) $E_f < E$.](image)
Two-dimensional Theories of Nanosized Plates and Shells

The theory of elasticity with surface stresses is applied to the modifications of the two-dimensional theories of nanosized plates and shells:

- Miller & Shenoy (2000);
- Dahmen, Lehwald & Ibach (2000);
- Lu, He, Lee & Lu (2006);
- Huang (2008);
- Lu, Lim & Chen (2009);
- Eremeyev, Altenbach & Morozov (2009a,b, 2010, 2012);

Various theories of plates are formulated, i.e. Kirchhoff–Love, Reissner & Mindlin, von Kàrmàn, and the 6-parameters theory by Libai & Simmonds among others.
Shell-like body
3D to 2D Reduction

\[ T^* = T + T_S, \quad M^* = M + M_S, \]
2D equilibrium equations

\[ \nabla_S \cdot T + q = 0, \quad \nabla_S \cdot M + T_\times + m = 0, \]

where \( T \) and \( M \) are the stress resultant and stress couple tensors, respectively, \( q \) and \( m \) are the external surface loads and moments, and \( T_\times \) denotes the vectorial invariant of the second-order tensor \( T \).

\[
T = \left\langle (A - zB)^{-1} \cdot \sigma \right\rangle + S_+ + S_-, \quad \left\langle (\ldots) \right\rangle = \int_{-h/2}^{h/2} (\ldots) G \, dz,
\]

\[
M = -\left\langle (A - zB)^{-1} \cdot z\sigma \times n \right\rangle - \frac{h}{2}(S_+ - S_-) \times n,
\]

\[
q = G_+ \varphi_+ - G_- \varphi_-, \quad m = \frac{h}{2}G_+ n \times \varphi_+ + \frac{h}{2}G_- n \times \varphi_-,
\]

\[
G = G(z) \equiv \det(A - zB), \quad G_\pm = G(\pm h/2), \quad B = -\nabla_S n.
\]

If \( h\|B\| \ll 1 \) then

\[
T = \left\langle A \cdot \sigma \right\rangle + S_+ + S_-, \quad M = -\left\langle A \cdot z\sigma \times n \right\rangle - \frac{h}{2}(S_+ - S_-) \times n.
\]
2D constitutive equations

Kinematic assumptions

$$u(q^1, q^2, z) = w(q^1, q^2) - z \vartheta(q^1, q^2), \quad n \cdot \vartheta = 0.$$ 

Constitutive relations

$$T = C_1 E + C_2 A_{tr} E + \Gamma \gamma \otimes n, \quad M = - [D_1 K + D_2 A_{tr} K] \times n,$$

where $E$, $K$, and $\gamma$ are the surface strain measures given by

$$E = \frac{1}{2} \left( \nabla_S w \cdot A + A \cdot (\nabla_S w)^T \right), \quad K = \frac{1}{2} \left( \nabla_S \vartheta \cdot A + A \cdot (\nabla_S \vartheta)^T \right),$$

$$\gamma = \nabla_S (w \cdot n) - \vartheta,$$

$C_1, C_2$ are the tangential stiffness parameters, $D_1$ and $D_2$ are the bending stiffness parameters, and $\Gamma$ is the transverse shear stiffness.
Stiffness parameters

\[ C_1 = 2C_{22} + 4\mu_S, \quad C_2 = C_{11} - C_{22} + 2\lambda_S, \]
\[ D_1 = 2D_{22} + h^2\mu_S, \quad D_2 = D_{33} - D_{22} + \frac{h^2}{2}\lambda_S, \quad \Gamma = \ell^2D_{22}, \]
\[ C_{11} = \frac{1}{2}\left(\frac{2E_fh_f}{1 - \nu_f} + \frac{E_h}{1 - \nu}\right), \quad C_{22} = \frac{1}{2}\left(\frac{2E_fh_f}{1 + \nu_f} + \frac{E_h}{1 + \nu}\right), \]
\[ D_{22} = \frac{1}{24}\left[\frac{E_f(h^3 - h^3_c)}{1 + \nu_f} + \frac{E_h^3}{1 + \nu}\right], \quad D_{33} = \frac{1}{24}\left[\frac{E_f(h^3 - h^3_c)}{1 - \nu_f} + \frac{E_h^3}{1 - \nu}\right], \]

where \(\ell\) is the minimal positive root of the following equation

\[ \mu_0 \cos \ell \frac{h_f}{2} \cos \ell \frac{h_c}{2} - \sin \ell \frac{h_f}{2} \sin \ell \frac{h_c}{2} = 0, \quad \mu_0 = \frac{\mu_c}{\mu_f}, \]

\(\mu\) and \(\mu_f\) are the shear moduli of the shell core and faces, respectively.
Tangential and bending stiffness

The effective tangential and bending stiffness take the form

\[ C^* \equiv C_1 + C_2 = \frac{2E_f h_f}{1 - \nu_f^2} + \frac{Eh_c}{1 - \nu^2} + 4\mu_S + 2\lambda_S, \]

\[ D^* \equiv D_1 + D_2 = \frac{1}{12} \left[ \frac{E_f(h^3 - h_c^3)}{1 - \nu_f^2} + \frac{Eh_c^3}{1 - \nu^2} \right] + \frac{h^2}{2}(2\mu_S + \lambda_S). \]

The classical bending stiffness \( D \) and the bending stiffness of the three-layered plate \( D_l \) are given by

\[ D = \frac{Eh^3}{12(1 - \nu^2)}, \quad D_l = \frac{1}{12} \left[ \frac{E_f(h^3 - h_c^3)}{1 - \nu_f^2} + \frac{Eh_c^3}{1 - \nu^2} \right], \]

and is assumed to be \( E_f > E \).
Bending stiffness

\[ D^* \] \hspace{1cm} D^* \hspace{1cm} D_l \hspace{1cm} D \]

0 \hspace{1cm} d \hspace{1cm} h_f \hspace{1cm} 2h_f \hspace{1cm} h
Bending Stiffness

\[ D \equiv D_1 + D_2 = D_\infty + D_{\text{surface}}, \]
\[ D_\infty = \frac{Eh^3}{12(1 - \nu^2)}, \quad D_{\text{surface}} = h^2(\mu^S + \lambda^S/2) \]

(2)

From the positivity of the surface energy density it follows

\[ \mu_S > 0, \quad \mu_s + \lambda_S > 0 \quad \Rightarrow \quad D_{\text{surface}} > 0 \]

\[ \frac{D}{D_\infty} \sim \frac{1}{h}, \quad h \to 0 \]
Bending Stiffness of a Plate made of Al

\[ \frac{D}{D_{\infty}} \]

\[ \mu = 34.7 \text{ GPa}, \quad \nu = 0.3 \]

\[ \chi^S = -3.48912 \text{ N/m}, \quad \mu^S = 6.2178 \text{ N/m} \]
Stiffness Parameters $\bar{C}_1 = C_1/C(1-\nu)$, $\bar{C}_2 = C_2/C\nu$,

$\bar{D}_1 = D_1/D(1-\nu)$, $\bar{D}_2 = D_2/D\nu$
Homogenization+Homogenization: two steps of Homogenization

On effective surface properties

- Find 2D effective (apparent) material properties.

On effective bulk properties

- Using these 2D properties find 3D effective material properties.
“Foam-like” surface

ZnO nanofoam grown on the glass substrate.
Effective properties for “foam-like” surface

On effective bulk properties
Following Gibson and Ashby (1997)

\[
\frac{E_f}{E_b} \sim \alpha^m, \quad \frac{G_f}{G_{sb}} \sim \alpha^m,
\]

where \(\alpha\) is the porosity, \(m \approx 2\), \(\nu_f \approx 0.3\)

On effective bulk properties at the nanoscale
Following Wang et al. (2006) we assume the scaling law

\[
E_n = E_s \left(1 + \chi \frac{l_{in}}{R}\right),
\]

where \(l_{in}\) an intrinsic length scale related to the surface properties, \(R\) is the specimen size, and \(\chi\) a nondimensional constant.
Effective properties for “foam-like” surface. II

**Scaling law**

We modify the dependence of the elastic moduli of a nanofoam on the porosity by the law

\[
\frac{E_{np}}{E_b} \sim \left(1 + \chi \frac{l_{in}}{R}\right) \alpha^m, \quad \frac{G_{np}}{G_b} \sim \left(1 + \chi \frac{l_{in}}{R}\right) \alpha^m,
\]

where \(E_{np}\) and \(G_{np}\) are the Young’s and shear moduli of a nanofoam, respectively. \(l_{in}\) is related to the surface effects and is typically in the order of \(0.01 – 0.1\)nm, see Duan et al. (2008), Wang et al. (2006).
Array of fibers

$d_f$ and $h_f$ are the diameter and height, $N$ denotes the number of fibers per unit area.
“Averaged” properties of layer of fibers

A transversely isotropic material

The longitudinal Young’s modulus

\[ E_\perp = N C_f. \]

The in-plane shear modulus

\[ G_f = \frac{12N}{h_f^2} D_f. \]

Other three elastic moduli are determined by interaction forces between fibers, that is adhesion-type forces.

\[ C_f = \frac{\pi d_f^2}{4} E_f \] and \( D_f \) are the tangential and bending stiffness of the fiber.
Conclusions and Future Steps

- We discussed the effective surface properties taking into account the surface stresses.
- We found the few expressions for effective stiffness parameters of plates and shells.
- In particular, the bending stiffness is bigger for the shells with surface stresses than for shells without surface elasticity.
- The surface residual stresses influence the effective stiffness parameters making the body more or less stiffer.
- Inner structure of the “surface” leads to changes in effective properties of materials at the nano- and microscales.
References

Thank you for your attention!!!

Further questions:

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