Surface Energy, Elasticity and the Homogenization of Rough Surfaces

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Abstract

Due to a larger surface to volume ratio, phenomena at the nanoscale require consideration of surface energy effects and the latter are frequently used to interpret size-effects in material behavior. Extensive work exists on deriving homogenized constitutive responses for macroscopic composites—relating effective properties to various microstructural details. In the present work, we focus on homogenization of *surfaces*. Indeed, elucidation of the effect of surface roughness on the surface energy, stress and elastic behavior is relatively under-studied and quite relevant to the behavior of nanostructures. We present derivations that relate both periodic and random roughness to the effective surface elastic behavior. We find that the residual surface stress is hardly affected by roughness while the superficial elastic properties are dramatically altered and, importantly, they may also change sign—this has significant ramifications in the interpretation of sensing based on frequency measurement changes. Interestingly, even if the bare surface has a zero surface elasticity modulus, roughness is seen to endow it with one. Using atomistic calculations, we verify the qualitative validity of the obtained theoretical insights. We show, through an illustrative example, that the square of resonance frequency of a cantilever beam with rough surface can decrease almost by a factor of two compared to a flat surface.

1 Introduction

For a cubic piece of copper with 1 nm sides, nearly 64% of the atoms reside on the surface. This simple fact makes apparent the enormous role surfaces play at the nanoscale. Surface atoms have different coordination numbers, charge distribution and subsequently different physical, mechanical and chemical properties. These differences are manifested phenomenologically in that the various bulk properties such as elastic modulus, melting temperature, electromagnetic properties among

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others are different for surfaces. For example, experiments show that some surfaces are elastically softer (Goudeau et al., 2001; Hurley et al., 2001; Villain et al., 2002; Sun and Zhang, 2003; Workum and Pablo, 2003), while others stiffer (Renault et al., 2003). These differences play an increasing role as the material characteristic size is shrunk smaller and smaller e.g. leading to size-dependency in the elastic modulus of nanostructures.

Surface energy effects are usually accounted via recourse to a theoretical framework proposed by Gurtin and Murdoch (1975, 1978). The surface is treated as a zero-thickness deformable elastic entity possessing non-trivial elasticity as well as a residual stress (the so-called "surface stress"). It is worthwhile to indicate that while fundamentally similar, a parallel line of works exist that are more materials oriented: Cahn (1989), Streitz (1994), Weissmuller and Cahn (1997), Johnson (2000), Voorhees and Johnson (2004) and Cammarata (1994, 2009a, 2009b) among others. The reader is referred to an extensive recent review by Cammarata (2009) on the literature. Steigmann and Ogden (1997) later generalized the Gurtin-Murdoch theory and incorporated curvature dependence of surface energy, thus resolving some important issues related to the use of Gurtin-Murdoch theory in the context of compressive stress states and for wrinkling type behavior. A few recent works have theoretically and atomistically examined the importance of the Steigmann-Ogden generalization (see for example, Fried and Todres, 2005; Schiavone and Ru, 2009, Chhapadia et. al., 2011a,b, Mohammadi and Sharma, 2012).

The ramifications of surface-energy related size-effects have been examined in several contexts, e.g. nanoinclusions (Duan et al., 2005a, 2005b; He and Li, 2006; Lim et al., 2005; Hui and Chen, 2010; Mi and Kouris 2007; Sharma et al. 2003, Sharma and Ganti, 2004; Sharma and Wheeler, 2007; Tian and Rajapakse, 2007, 2008), quantum dots (Sharma et al. 2002, 2003; Peng et al., 2006), nanoscale beams and plates (Miller and Shenoy, 2000; Jing et al. 2006; Bar et al. 2010; Liu and Rajapakse, 2010; Liu et. al., 2011), nano-particles, wires and films (Streitz et al. 1994; Diao et al. 2003, 2004; Villain et al., 2004; Dingreville et al., 2005; Diao et al., 2006), sensing and vibration (Lim and He, 2004; Wang and Feng, 2007; Park and Klein, 2008; Park, 2009), composites (Mogilevskaya et al., 2008). The following papers have focused on calculation of surface properties from atomistics: Shenoy, 2005; Shodja and Tehranchi, 2010; Mi et al., 2008, Chhapadia et. al., 2011a,b, Mohammadi and Sharma, 2012).

Some recent works are worth mentioning as they provide clarifications and guidance on the theories underlying surface energy effects, e.g. Ru (2010), Mogielvskaya (2008, 2010) and Schiavone and Ru (2009). The papers by Wang et al. (2010) and Huang and Sun (2007) have pointed out the importance of residual surface stress on the elastic properties of nanostructures and composites.

Surfaces of real materials, even the most thoroughly polished ones, will typically exhibit random roughness across different lateral length scales. How are the surface properties renormalized due to such roughness? Can the surface roughness be artificially tailored to obtain desired surface characteristics? These questions are at the heart of the present manuscript. We provide a homogenization scheme for both periodically and randomly rough surface duly incorporating both surface stress and surface elasticity. Very little work has appeared that addresses effect of roughness on both surface stress and surface elasticity. Notable exceptions are the following recent works: Wiessmuller and Duan (2008) who focus on deriving the effective residual stress for the rough surface of a cantilever beam and their follow-up work by Wang et al., (2010) who generalized it to the anisotropic case. We will briefly comment on their in the discussion section. One specific difference is that we also derive effective superficial elasticity constants and not just the residual surface stress. The outline of this paper is as follows. In Section 2 we briefly summarize the Gurtin-Murdoch surface elasticity theory and formulate the problem while in Section 3 we present our general homogenization strategy. In Section 4, specializing to the 2D case, we present results for both randomly and periodically rough surfaces. Discussion of our results is in Section 5 where present results of our atomistic calculations designed to check the qualitative correctness of the theoretical predictions and point out the implications for nano-cantilever-beam based sensing.

Notation. We will employ both direct and index notion: vectors and tensors are represented by bold symbols, e.g., $\mathbf{a}$, $\mathbf{T}$, etc, and in index notation the corresponding components are denoted by a_i, T_{ij}, etc with the canonical basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ tacitly understood. Summation over repeated index is followed unless otherwise stated. The basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are also written as $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ and the associated spatial coordinates are either denoted by (x_1, x_2, x_3) or (x, y, z). Partial derivatives with respect to spatial variable x_i is sometimes denoted by $(\ )_{,i}$. The inner (dot) product between two matrix of the same size $\mathbf{A}$ and $\mathbf{B}$ is defined as $\mathbf{A} \cdot \mathbf{B} = \mathrm{Tr}(\mathbf{A}\mathbf{B}^T) = A_{pi}B_{pi}$.

We also collect some useful relations pertaining to calculus on surfaces. Let $B \subset \mathbb{R}^3$ be a regular simply connected domain, $\mathbf{t}_n$ be the unit outward normal on ∂B (cf., Fig. 1(a)), $\mathbf{I}$ be the identity mapping from $\mathbb{R}^3$ to $\mathbb{R}^3$, and

$$\mathbb{P} = \mathbf{I} - \mathbf{t}_n \otimes \mathbf{t}_n \tag{1.1}$$

be the projection from $\mathbb{R}^3$ to the tangential subspace $\mathcal{T} := \{\mathbf{a} \in \mathbb{R}^3 : \mathbf{a} \cdot \mathbf{t}_n = 0\}$ at a point $\mathbf{p} \in \partial B$. Let $\varphi : B \to \mathbb{R}$ be a scalar field, $\mathbf{u} : B \to \mathbb{R}^3$ a vector field, and $\mathbf{T} : B \to \mathrm{Lin}(\mathbb{R}^3, \mathbb{R}^3) := \{\mathbf{M} : \mathbb{R}^3 \to \mathbb{R}^3 \text{ is linear}\}$ be a tensor field. Suppose that $\varphi, \mathbf{u}, \mathbf{T}$ are differentiable up to the boundary ∂B. Then the surface gradient of φ and $\mathbf{u}$ can be defined as

$$\nabla_s \varphi = \mathbb{P}\nabla\varphi, \qquad \nabla_s \mathbf{u} = (\nabla \mathbf{u})\mathbb{P},$$

where the convention $(\nabla \mathbf{u})_{pi} = \partial_{x_i}(\mathbf{u})_p$ is followed. If, in particular, $\mathbf{u} : B \to \mathbb{R}^3$ is the displacement, then the *surface strain* is defined as

$$\mathbf{E}_s = \mathbb{P}\mathbf{E}\mathbb{P} = \frac{1}{2}[\mathbb{P}\nabla_s \mathbf{u} + (\mathbb{P}\nabla_s \mathbf{u})^T] \qquad \text{on } \partial B, \tag{1.2}$$

which measures the deformation within the surface ∂B. Also, we have the following identities (or definitions) from Gurtin and Murdoch (1975):

$$\begin{cases} \mathrm{div}_s \mathbf{u} = \mathrm{Tr}(\mathbb{P}\nabla_s \mathbf{u}), & \mathbf{a} \cdot (\mathrm{div}_s \mathbf{T}) = \mathrm{div}_s(\mathbf{T}^T \mathbf{a}) \quad \forall \mathbf{a} \in \mathbb{R}^3, \\ \mathrm{div}_s(\varphi \mathbf{u}) = \varphi \nabla_s \mathbf{u} + \mathbf{u} \cdot \nabla_s \varphi, & \mathrm{div}_s(\varphi \mathbf{T}) = \varphi \mathrm{div}_s \mathbf{T} + \mathbf{T}\nabla_s \varphi. \end{cases} \tag{1.3}$$

Let $C \subset \partial B$ be a simple contour, $\boldsymbol{\nu} \in \mathcal{T}$ be the unit outward normal on C, and $S_C \subset \partial B$ be the surface enclosed by C (cf., Fig. 1(b)). In analogy with the classic divergence theorem, if the vector field $\mathbf{u}$ is tangential on ∂B and differentiable we have

$$\int_{S_C} \mathrm{div}_s \mathbf{u} = \int_C \mathbf{u} \cdot \boldsymbol{\nu},$$

Applying the above identity to $\mathbf{T}^T \mathbf{a}$ for a differentiable tensor field $\mathbf{T}(\mathbf{x}) : \mathcal{T} \to I\!R^3$, by (1.3) we obtain

$$\int_{S_C} \mathrm{div}_s \mathbf{T} = \int_C \mathbf{T}\boldsymbol{\nu}, \tag{1.4}$$

which will be critical for deriving the local form of the equilibrium equation on the surface.

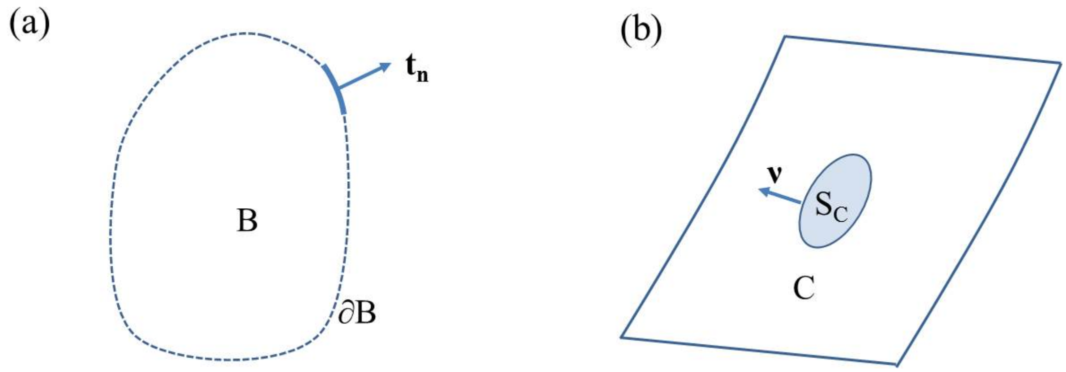

Figure 1: (a) An elastic body $B \subset \mathbb{R}^3$ with surface ∂B and unit outward normal $\mathbf{t}_n$, and (b) the subsurface $S_C \subset \partial B$ enclosed by a simple contour C with unit outward normal $\boldsymbol{\nu}$ within the surface.

2 Surface Elasticity

Let $B \subset \mathbb{R}^3$ be a regular domain occupied by an elastic body, $\mathbf{C}: \mathbb{R}^{3\times 3} \to \mathbb{R}^{3\times 3}$ be the fourth-order bulk stiffness tensor of the elastic medium. In linearized elasticity and in the absence of applied body force, the displacement $\mathbf{u} : B \to \mathbb{R}^3$ satisfies the equilibrium equation

$$\mathrm{div}(\mathbf{C}\nabla\mathbf{u}) = 0 \qquad \text{in } B. \tag{2.1}$$

Appropriate boundary conditions on ∂B are necessary for solving the above equations which we describe below in detail.

We employ the linearized surface elasticity theory of Gurtin and Murdoch (Gurtin and Murdoch, 1975; Gurtin et. al., 1998). In this theory the surface is modeled as a deformable elastic membrane adhering to the bulk material without slipping. From (1.2), we see that surface strains belong to the following subspace

$$\mathbb{M} = \{\mathbf{M} \in \mathrm{Lin}(\mathbb{R}^3, \mathbb{R}^3) : \ \mathbf{M}\mathbf{t}_n = 0, \ \mathbf{M}^T = \mathbf{M}\}. \tag{2.2}$$

Let $\tau^0 \in \mathbb{R}$ be the magnitude of the residual isotropic stress tensor and $\mathbf{I}_s = \mathbb{P}$ be the identity mapping from the tangential space $\mathcal{T}$ to $\mathcal{T}$. We adopt the linear isotropic surface constitutive law from Gurtin and Murduch (1975), equation (8.6), i.e., for given displacement $\mathbf{u} : B \to \mathbb{R}^3$ the surface stress is given by

$$\mathbf{S}_s = \mathbf{C}_s\nabla\mathbf{u} + \mathbf{S}_s^0 = \mathbf{C}_s\mathbf{E}_s + \mathbf{S}_s^0 \qquad \text{on } \partial B \tag{2.3}$$

where $\mathbf{S}_s^0 = \tau^0\mathbf{I}_s$ is the residual surface stress tensor, the forth-order symmetric surface stiffness tensor $\mathbf{C}_s : \mathbb{R}^{3\times 3} \to \mathbb{R}^{3\times 3}$ is such that

$$\mathbf{C}_s(\mathbf{H}) = 2\mu^s\mathbb{P}\mathbf{E}\mathbb{P} + \lambda^s\mathrm{Tr}(\mathbb{P}\mathbf{E}\mathbb{P})\mathbf{I}_s, \quad \mathbf{E} = \frac{1}{2}(\mathbf{H} + \mathbf{H}^T), \qquad \forall\, \mathbf{H} \in \mathbb{R}^{3\times 3}, \tag{2.4}$$

and μ^s, λ^s are the surface elastic constants in analogy with the bulk Lamé constants.

We remark that the above surface stiffness tensor $\mathbf{C}_s$ is assumed to be independent of the normal direction of the surface. This is not true for crystalline surfaces but facilitates analytical results in the same vein as the frequent use of the assumption of isotropy for bulk elasticity. Also, the surface constitutive law (2.3) is different from that of Gurtin and Murdoch (1975) by a term of $\tau^0\nabla_s\mathbf{u}$. This term leads to asymmetry of the surface stress tensor and quite a few works have chosen to ignore its presence completely (as justified in some cases). The reader is referred to Ru (2010), Mogilevskaya et al. (2008) and Huang (2010) for further discussions on this subject. We have chosen to neglect this term. A simple calculation (not presented in this manuscript) confirmed that the effect of this term is small in the present context.

In the absence of applied traction on ∂B, the equilibrium of any sub-surface $S_C \subset \partial B$ implies that (cf., Fig. 1 (b))

$$\int_C \mathbf{S}_s \boldsymbol{\nu} + \int_{S_C} (\mathbf{C}\nabla\mathbf{u})(-\mathbf{t}_n) = 0, \quad \text{i.e.,} \quad (\mathbf{C}\nabla\mathbf{u})\mathbf{t}_n = \mathrm{div}_s[\mathbf{C}_s\nabla\mathbf{u} + \mathbf{S}_s^0] \qquad \text{on } \partial B, \tag{2.5}$$

where div_s denotes surface divergence. The above equations are a generalization of the classic Young-Laplace equation and also serve as boundary conditions for (2.1). In summary, equations (2.1) and (2.5) consitute the boundary value problem for linearized elasticity with surface elastic effects.

Further, it is worthwhile to note that equations (2.1) and (2.5) are also the Euler-Lagrange equation of the variational principle:

$$\min_{\mathbf{u}} \left\{ U[\mathbf{u}] := \frac{1}{2}\int_B \nabla\mathbf{u}\cdot\mathbf{C}\nabla\mathbf{u} + \Gamma[\mathbf{u}] \right\}, \tag{2.6}$$

where $\Gamma[\mathbf{u}]$ denotes the elastic energy contributed by the surface (Gurtin and Murdoch, 1975, equation 9.3 and theorem 9.1):

$$\Gamma[\mathbf{u}] = \int_{\partial B} \left[\frac{1}{2}\nabla\mathbf{u}\cdot\mathbf{C}_s\nabla\mathbf{u} + \nabla\mathbf{u}\cdot\mathbf{S}_s^0 + \gamma \right]. \tag{2.7}$$

Here the constant γ measures the energy cost of creating a free surface and has no effect on (2.1) and (2.5). This is the surface energy in the absence of surface strain and may be linked to fracture toughness. The existence and uniqueness of solutions to (2.6) can be similarly discussed as for bulk elasticity based on the algebraic properties of tensors $\mathbf{C}$ and $\mathbf{C}_s$ (Altenbach *et al.*, 2011).

3 Homogenization Strategy and Problem Formulation

In this section we outline our homogenization strategy for a rough surface, formulate the problem and sketch out the solution method.

As illustrated in Fig. 2, we consider a semi-infinite elastic body with $B = \{(x, y, z) : y < h(x, z)\}$, where the function $h(x, z)$ describes the surface roughness. Assume that the amplitude of the roughness h is small compared with the length scale of the overall bulk body: $h \sim \delta \ll 1 \sim$ length scale of the bulk body. The number δ will be the small parameter used in our subsequent perturbation calculations. The overall half space is subject to a uniform in-plane far applied stress $\mathbf{CH}^\infty$ where $\mathbf{H}^\infty \in \mathbb{R}^{3\times3}$ is the corresponding far-field strain. By (2.1) and (2.5) our original problem is to solve for $\mathbf{u} : B \to \mathbb{R}^3$.

$$\begin{cases} \mathrm{div}(\mathbf{C}\nabla\mathbf{u}) = 0 & \text{in } \ B, \\ (\mathbf{C}\nabla\mathbf{u})\mathbf{t}_n = \mathrm{div}_s(\mathbf{C}_s\nabla\mathbf{u} + \mathbf{S}_s^0) & \text{on } \ \partial B, \\ \nabla\mathbf{u} \to \mathbf{H}^\infty & \text{as } \ |y| \to \infty. \end{cases} \tag{3.1}$$

The boundary condition $(3.1)_2$, for a rough surface ∂B, prevents an exact solution and accordingly we will take recourse in the formal perturbation method. Assume that the solution to (3.1) can be expanded as

$$\mathbf{u} = \mathbf{u}^{(0)} + \delta\mathbf{u}^{(1)} + \delta^2\mathbf{u}^{(2)} + \cdots. \tag{3.2}$$

Inserting (3.2) into (3.1), by $(3.1)_1$ and $(3.1)_3$ we have

$$\begin{cases} \operatorname{div}[\mathbf{C}\nabla\mathbf{u}^{(i)}] = 0 \quad (i=0,1,2) & \text{in } B^0, \\ \nabla\mathbf{u}^{(0)} \to \mathbf{H}^\infty, \quad \nabla\mathbf{u}^{(i)} \to 0 \quad (i=1,2) & \text{as } |y| \to \infty, \end{cases} \tag{3.3}$$

where $B^0 = \{(x,y,z) : y < 0\}$ is the half space with a flat surface.

The boundary conditions on the rough surface, i.e., $(3.1)_2$, can be converted to an effective boundary condition on the nominal flat surface ∂B^0. To this end, we assume that the displacement on ∂B can be obtained by extrapolating from the displacement and their derivatives on ∂B^0 through Taylor series expansion. Upon tedious calculations presented in § 4.1, we find the boundary conditions on the nominal flat surface as

$$(\mathbf{C}\nabla\mathbf{u}^{(i)})\mathbf{e}_2 = \mathbf{p}^{(i)} \quad (i=0,1,2) \qquad \text{on } \partial B^0, \tag{3.4}$$

where the detailed expressions for surface traction $\mathbf{p}^{(i)}$ are presented in § 4.1. We recognize that the boundary value problems specified by (3.3) and (3.4) for $\mathbf{u}^{(i)}$ are the classical Cerruti-Boussinesq half-space problems whose solutions can be found in textbooks, e.g., Johnson (1985).

Once the local stress and strain are found, we can calculate the total elastic energy of the half-space in the presence of the rough surface as a function of the far applied strain $\mathbf{H}^\infty$:

$$E^{\mathrm{act}}(\mathbf{H}^\infty) = \frac{1}{2}\int_B \left[\nabla\mathbf{u}\cdot\mathbf{C}\nabla\mathbf{u} - \nabla\mathbf{u}^{(0)}\cdot\mathbf{C}\nabla\mathbf{u}^{(0)}\right] + \int_{\partial B}\left[\frac{1}{2}\nabla\mathbf{u}\cdot\mathbf{C}_s\nabla\mathbf{u} + \nabla\mathbf{u}\cdot\mathbf{S}_s^0 + \gamma\right], \tag{3.5}$$

where the bulk energy for flat surface is subtracted to avoid unbounded integrals. The total elastic energy E^{act} depends on the far applied strain $\mathbf{H}^\infty$ since $\mathbf{u} \approx \mathbf{u}^{(0)} + \delta\mathbf{u}^{(1)} + \delta^2\mathbf{u}^{(2)}$ according to (3.2), and $\mathbf{u}^{(k)}$ $(k=0,1,2)$ being the solution of (3.1) and (3.4) depends on the far applied strain $\mathbf{H}^\infty$. We remark that the first and second term on the right hand side of (3.5) are the elastic energy contributed by the bulk and surface, respectively.

We will approximate rough-surface elastic body by a half-space solid with a flat surface where the flat surface has effective properties different from the original rough surface. To define the effective properties of the surface, we propose to equate the total elastic energy of the rough-surface half space (E^{act}) to the total elastic energy of a half space with a nominal effective flat surface (E^{eff}):

$$E^{\mathrm{act}}(\mathbf{H}^\infty) = E^{\mathrm{eff}}(\mathbf{H}^\infty), \tag{3.6}$$

where

$$E^{\mathrm{eff}}(\mathbf{H}^\infty) = \int_{\partial B^0}\left[\frac{1}{2}\nabla\mathbf{u}^{(0)}\cdot\mathbf{C}_s^{\mathrm{eff}}\nabla\mathbf{u}^{(0)} + \nabla\mathbf{u}^{(0)}\cdot(\mathbf{S}_s^0)^{\mathrm{eff}} + \gamma^{\mathrm{eff}}\right], \tag{3.7}$$

$(\mathbf{S}_s^0)^{\mathrm{eff}}$ is the effective surface residual stress, $\mathbf{C}_s^{\mathrm{eff}}$ is the effective surface elasticity tensor, and γ^{eff} the effective surface energy density in the absence of surface strain. The bulk energy term has been subtracted from (3.7) in analogy with (3.5).

4 Solutions

4.1 Boundary conditions for perturbed solutions

We now specialize to two dimensions, assuming the body is infinite in $-\mathbf{e}_y$-direction, $\pm\mathbf{e}_x$-directions, and in either plane strain state ($\varepsilon_{zz} = \varepsilon_{zx} = \varepsilon_{zy} = 0$) or plane stress state ($\sigma_{zz} = \sigma_{zx} = \sigma_{zy} = 0$).

For isotropic materials, the stress-strain relations for plane problems are given by:

$$\begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{xy} \end{bmatrix} = \mathbf{L} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{bmatrix}, \qquad \mathbf{L} = \begin{bmatrix} L_{11} & L_{12} & 0 \\ L_{12} & L_{11} & \\ 0 & 0 & L_{33} \end{bmatrix}, \tag{4.1}$$

where the 3×3 matrix $\mathbf{L}$, formed by elastic constants, are given by (E – Young's modulus, μ – shear modulus, ν – Poisson's ratio):

$$\mathbf{L} = \frac{1}{2\mu} \begin{bmatrix} 1-\nu & -\nu & 0 \\ -\nu & 1-\nu & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ (plane strain)} \quad \text{or} \quad \frac{1}{E} \begin{bmatrix} 1 & -\nu & 0 \\ -\nu & 1 & 0 \\ 0 & 0 & (1+\nu) \end{bmatrix} \text{ (plane stress)}. \tag{4.2}$$

Our work can be readily extended to three dimensions. However, the calculations are quite tedious with relatively little prospects for (additional) novel insights. We will employ two coordinate systems. The first one is the canonical Cartesian frame $(\mathbf{e}_1, \mathbf{e}_2)$ parallel and perpendicular to the nominally flat surface while the second one $(\mathbf{t}_1, \mathbf{t}_2)$ is the unit normal and unit tangent along the curve, see Fig. 2. Assume that the surface is parameterized by $y = \delta h_0(x)$ $(\delta << 1)$. It is easy to show that the transformations between the moving curvilinear frame $(\mathbf{t}_1, \mathbf{t}_2)$ and fixed Cartesian frame $(\mathbf{e}_1, \mathbf{e}_2)$ are given by

$$\mathbf{t}_k = (\mathbf{M})_{ki}\mathbf{e}_i, \qquad \mathbf{e}_i = (\mathbf{N})_{ik}\mathbf{t}_k, \tag{4.3}$$

where ($\Gamma(\delta, x) = \sqrt{1 + \delta^2 h_{0x}^2}$, $\mathbf{I}$ is now the 2×2 identity matrix)

$$\begin{aligned} &\mathbf{M} = \frac{1}{\Gamma(\delta,x)} \begin{bmatrix} 1 & \delta h_{0x} \\ -\delta h_{0x} & 1 \end{bmatrix} = \mathbf{I} + \delta \mathbf{W} - \frac{1}{2}\delta^2 h_{0x}^2 \mathbf{I} + o(\delta^2), \qquad \mathbf{W} = \begin{bmatrix} 0 & h_{0x} \\ -h_{0x} & 0 \end{bmatrix}, \\ &\mathbf{N} = \mathbf{M}^T = \mathbf{M}^{-1} = \mathbf{I} - \delta \mathbf{W} - \frac{1}{2}\delta^2 h_{0x}^2 \mathbf{I} + o(\delta^2), \\ &h_{0x} = \partial_x h_0(x) \quad \text{(likewise, } h_{0xx} = \partial_{xx} h_0(x), \ h_{0xxx} = \partial_{xxx} h_0(x), \text{ etc).} \end{aligned} \tag{4.4}$$

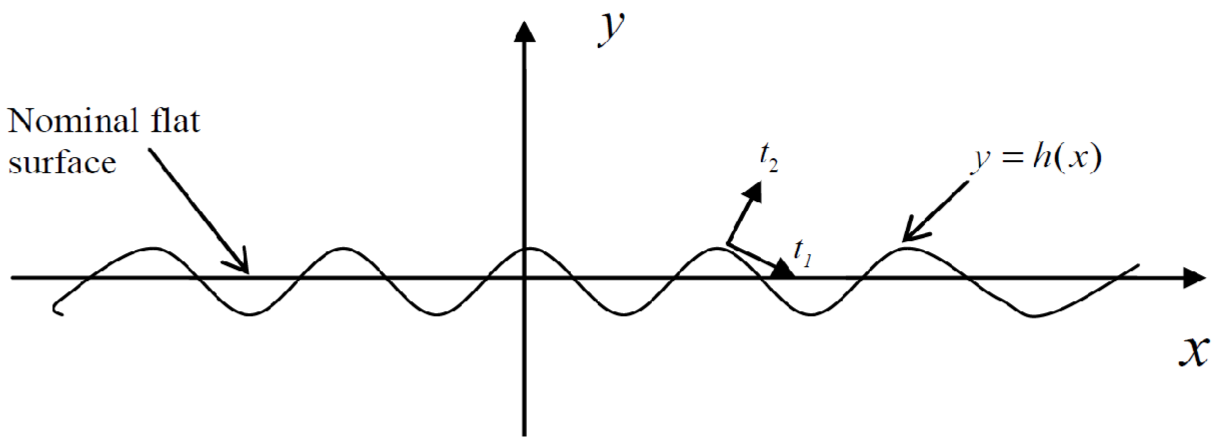

Figure 2: A rough surface profile

To address the effects of rough surface and surface elasticity, we have assumed formal expansion (3.2) of the solution to (3.1). To solve for $\mathbf{u}^{(i)}$ $(i = 0, 1, 2)$, we need to convert the original boundary conditions $(3.1)_2$ into boundary conditions on the nominal flat surface ∂B^0. To this end, we further assume that the displacement around the nominal flat surface ∂B^0 (i.e., $|y| \sim \delta$) is given by

$$\mathbf{u}(x,y) = \mathbf{u}(x,0) + y\partial_y \mathbf{u}(x,0) + \frac{1}{2}y^2 \partial_{yy}\mathbf{u}(x,0) + o(\delta^3). \tag{4.5}$$

Therefore, around the nominal flat surface ∂B^0 (i.e., $|y| \sim \delta$), by (4.5) the displacement gradient is given by

$$\mathbf{H} := \nabla \mathbf{u} = \mathbf{H}^0 + \delta \mathbf{H}^1 + \delta^2 \mathbf{H}^2 + o(\delta^2), \tag{4.6}$$

where

$$\begin{aligned} \mathbf{H}^0 &= [\partial_x \mathbf{u}^{(0)}, \partial_y \mathbf{u}^{(0)}], \qquad \mathbf{H}^1 = [\partial_x \mathbf{u}^{(1)}, \partial_y \mathbf{u}^{(1)}] + \frac{y}{\delta}[\partial_{xy}\mathbf{u}^{(0)}, \partial_{yy}\mathbf{u}^{(0)}], \\ \mathbf{H}^2 &= [\partial_x \mathbf{u}^{(2)}, \partial_y \mathbf{u}^{(2)}] + \frac{y}{\delta}[\partial_{xy}\mathbf{u}^{(1)}, \partial_{yy}\mathbf{u}^{(1)}] + \frac{y^2}{2\delta^2}[\partial_{xyy}\mathbf{u}^{(0)}, \partial_{yyy}\mathbf{u}^{(0)}]. \end{aligned} \tag{4.7}$$

In the above equations, the derivatives of $\mathbf{u}^{(i)}$ are evaluated at $y = 0$ and taken as column vectors, and hence $\mathbf{H}^i$ are 2×2 matrices. Recall that $\mathbf{t}_2 = \mathbf{e}_2 - \delta h_{0x}\mathbf{e}_1 - \frac{1}{2}\delta^2 h_{0x}^2 \mathbf{e}_2 + o(\delta^2)$ from (4.3)-(4.4). Then the left hand side of $(3.1)_2$ can be written as

$$\begin{aligned} (\mathbf{C}\nabla\mathbf{u})\mathbf{t}_2 = (\mathbf{C}\mathbf{H}^0)\mathbf{e}_2 &+ \delta[(\mathbf{C}\mathbf{H}^1)\mathbf{e}_2 - h_{0x}(\mathbf{C}\mathbf{H}^0)\mathbf{e}_1] \\ &+ \delta^2[(\mathbf{C}\mathbf{H}^2)\mathbf{e}_2 - h_{0x}(\mathbf{C}\mathbf{H}^1)\mathbf{e}_1 - \frac{1}{2}h_{0x}^2(\mathbf{C}\mathbf{H}^0)\mathbf{e}_2] + o(\delta^2) \qquad \text{on } \partial B. \end{aligned} \tag{4.8}$$

To calculate the expansion of the right hand side of $(3.1)_2$ with respect to δ, we first notice that

$$\mathbf{C}_s \nabla \mathbf{u} + \mathbf{S}_s^0 = \sigma_{ss}\mathbf{t}_1 \otimes \mathbf{t}_1 + \sigma_{33}\mathbf{e}_z \otimes \mathbf{e}_z \qquad \text{on } \partial B, \tag{4.9}$$

where

$$\begin{aligned} \sigma_{ss} &= \mathbf{t}_1 \cdot [\mathbf{C}_s(\mathbf{N}^T\mathbf{H}\mathbf{N})]\mathbf{t}_1 + \tau^0 =: \sigma_{ss}^0 + \delta\sigma_{ss}^1 + \delta^2\sigma_{ss}^2 + o(\delta^2), \\ \sigma_{ss}^0 &= \mathbf{t}_1 \cdot (\mathbf{C}_s\mathbf{H}^0)\mathbf{t}_1 + \tau^0, \qquad \sigma_{ss}^1 = \mathbf{t}_1 \cdot [\mathbf{C}_s(\mathbf{H}^1 + \mathbf{W}\mathbf{H}^0 + \mathbf{H}^0\mathbf{W}^T)]\mathbf{t}_1, \\ \sigma_{ss}^2 &= \mathbf{t}_1 \cdot [\mathbf{C}_s(\mathbf{H}^2 + \mathbf{W}\mathbf{H}^1 + \mathbf{H}^1\mathbf{W}^T - h_{0x}^2\mathbf{H}^0)]\mathbf{t}_1. \end{aligned} \tag{4.10}$$

Next, by the last of (1.3) and that σ_{33} is constant and hence $\mathrm{div}_s(\sigma_{33}\mathbf{e}_z \otimes \mathbf{e}_z) = 0$, we have

$$\mathrm{div}_s[\mathbf{C}_s\nabla\mathbf{u} + \mathbf{S}_s^0] = \sigma_{ss}[\mathbf{t}_1 \mathrm{div}_s \mathbf{t}_1 + (\nabla_s \mathbf{t}_1)\mathbf{t}_1] + \mathbf{t}_1(\mathbf{t}_1 \cdot \nabla_s \sigma_{ss}). \tag{4.11}$$

Recall the following identities from differential geometry:

$$\nabla_s \mathbf{t}_1 = [\delta h_{0xx} + o(\delta^2)]\mathbf{t}_2 \otimes \mathbf{t}_1, \qquad \mathrm{div}_s \mathbf{t}_1 = 0.$$

Therefore, by (4.3), (4.4) and (4.9) we find

$$\begin{aligned} \mathrm{div}_s[\mathbf{C}_s\nabla\mathbf{u} + \mathbf{S}_s^0] &= \delta\sigma_{ss}h_{0xx}\mathbf{t}_2 + \mathbf{t}_1(\mathbf{t}_1 \cdot \nabla_s\sigma_{ss}) \\ &= (\sigma_{ss}^0)_{,1}\mathbf{e}_1 + \delta\Big\{[(\sigma_{ss}^1)_{,1} + h_{0x}(\sigma_{ss}^0)_{,2}]\mathbf{e}_1 + [h_{0x}(\sigma_{ss}^0)_{,1} + \sigma_{ss}^0 h_{0xx}]\mathbf{e}_2\Big\} \\ &\quad + \delta^2\Big\{[(\sigma_{ss}^2)_{,1} - h_{0x}^2(\sigma_{ss}^0)_{,1} + h_{0x}(\sigma_{ss}^1)_{,2} - h_{0xx}h_{0x}\sigma_{ss}^0]\mathbf{e}_1 \\ &\quad + [h_{0x}(\sigma_{ss}^1)_{,1} + h_{0x}^2(\sigma_{ss}^0)_{,2} + \sigma_{ss}^1 h_{0xx}]\mathbf{e}_2\Big\} \qquad \text{on } \partial B. \end{aligned} \tag{4.12}$$

We remark that not all terms associated with δ^i $(i=0,1,2)$ contribute equally in regard of the fact that for typical solids,

$$\|\mathbf{C}\| >> \|\mathbf{C}_s\|k, \tag{4.13}$$

where $1/k$ is the typical wavelength of roughness profile $h_0(x)$ (i.e., the average distance between neighboring peaks or valleys). For example, copper has $\|\mathbf{C}\| \sim 10^{11}$ Pa while $\|\mathbf{C}_s\| \sim 1N/m$, and hence the above inequality is satisfied for typical solids up to atomistic scale. Enforcing (4.13) and neglecting lower order terms on the right hand side of (4.12), by (4.10) we have

$$\begin{aligned}\mathrm{div}_s[\mathbf{C}_s\nabla\mathbf{u}+\mathbf{S}_s^0] = \delta\Big\{&h_{0x}(\sigma_{ss}^0)_{,2}\mathbf{e}_1 + [h_{0x}(\sigma_{ss}^0)_{,1} + \sigma_{ss}^0 h_{0xx}]\mathbf{e}_2\Big\}\\ &+\delta^2[-h_{0x}^2(\sigma_{ss}^0)_{,1} - h_{0xx}h_{0x}\sigma_{ss}^0]\mathbf{e}_1 \qquad \text{on } \partial B.\end{aligned} \tag{4.14}$$

Comparing (4.8) with (4.14), by $(3.1)_2$ we find the boundary conditions for $\mathbf{u}^{(0)}$ are given by

$$(\mathbf{C}\nabla\mathbf{u}^{(0)})\mathbf{e}_2 = 0 \qquad \text{on} \qquad \partial B^0. \tag{4.15}$$

An obvious solution to the boundary value problem for $\mathbf{u}^{(0)}$, i.e., (3.3) and (4.15), is a uniform $\nabla\mathbf{u}^{(0)}$ such that

$$\mathbf{H}^0 = \nabla\mathbf{u}^{(0)} = \mathbf{H}^\infty. \tag{4.16}$$

By (4.7), we have

$$\nabla\mathbf{H}^0 = 0, \quad \mathbf{H}^1 = \nabla\mathbf{u}^{(1)}, \quad \mathbf{H}^2 = \nabla\mathbf{u}^{(2)} + h_0\partial_y\nabla\mathbf{u}^{(1)} \qquad \text{on } \partial B. \tag{4.17}$$

Moreover, comparing (2.3) with (2.4) we obtain the boundary conditions for $\mathbf{u}^{(2)}$:

$$(\mathbf{C}\nabla\mathbf{u}^{(1)})\mathbf{e}_2 = h_{0x}(\mathbf{C}\nabla\mathbf{u}_0)\mathbf{e}_1 + h_{0xx}\sigma_{ss}^0\mathbf{e}_2 =: \mathbf{p}^{(1)} \qquad \text{on } \partial B^0, \tag{4.18}$$

and

$$\begin{aligned}(\mathbf{C}\nabla\mathbf{u}^{(2)})\mathbf{e}_2 = -h_0\partial_y(\mathbf{C}\nabla\mathbf{u}^{(1)})\mathbf{e}_2 + h_{0x}(\mathbf{C}\nabla\mathbf{u}^{(1)})\mathbf{e}_1 + \frac{1}{2}h_{0x}^2(\mathbf{C}\nabla\mathbf{u}^{(0)})\mathbf{e}_2\\ -h_{0xx}h_{0x}\sigma_{ss}^0\mathbf{e}_1 =: \mathbf{p}^{(2)} \qquad \text{on } \partial B^0.\end{aligned} \tag{4.19}$$

In addition, we notice that the solutions to boundary value problems for $\mathbf{u}^{(i)} (i=1,2)$, i.e., (3.3) and (3.4) with $\mathbf{p}^{(i)}$ given by (4.18)-(4.19), are explicitly given by (A.1). Upon specifying the surface roughness profile $h_0(x)$, we can solve (3.3) and (3.4) for the elastic fields, compute the total elastic energy (3.5) and (3.7) and find the effective properties of the nominal flat surface according to (3.6). Below we present the detailed calculations for a sinusoidal surface and a random surface.

4.2 Sinusoidal roughness

To fix the idea we first consider a sinusoidal rough surface. Let the surface be described by $h(x) = \delta\cos(kx)$ $(\delta k \ll 1)$. This rough surface may be regarded as a perturbation of the flat surface ∂B^0:

$$h(x) = 0 + \delta\cos(kx) = \delta h_0(x), \qquad h_0 = \cos(kx), \qquad \delta k \ll 1 \tag{4.20}$$

Assume that the far applied stress is given by $\mathbf{C}\mathbf{H}^\infty = \varepsilon_{xx}^\infty / L_{11}\mathbf{e}_1 \otimes \mathbf{e}_1$, i.e., by (4.1),

$$\mathbf{H}^\infty = \varepsilon_{xx}^\infty \begin{bmatrix} 1 & 0 \\ 0 & \frac{L_{12}}{L_{11}} \end{bmatrix}. \tag{4.21}$$

The zeroth order strain is given by (4.16) and (4.21). By (4.18), we have

$$p_x^{(1)} = \alpha_1 \sin(kx), \qquad p_y^{(1)} = \beta_1 \cos(kx) \qquad \text{on } \partial B^0, \tag{4.22}$$

where $\alpha_1 = -k\varepsilon_{xx}^{\infty}/L_{11}$ and $\beta_1 = -k^2\sigma_{ss}^0 \approx -k^2\tau^0$ are constants. The first order stress field in B^0, determined by the boundary value problem (3.3) and (3.4), is given by (A.1):

$$\begin{aligned} \sigma_{xx}^{(1)} &= \big[\alpha_1(2+ky) + \beta_1(1+ky)\big]e^{ky}\cos(kx), \\ \sigma_{yy}^{(1)} &= -\big[\alpha_1 ky + \beta_1(ky-1)\big]e^{ky}\cos(kx), \\ \sigma_{xy}^{(1)} &= \big[\alpha_1(1+ky) + \beta_1 ky\big]e^{ky}\sin(kx). \end{aligned} \tag{4.23}$$

Therefore,

$$\begin{aligned} \varepsilon_{xx}^{(1)} &= \big[\alpha_1[2L_{11} + (L_{11}-L_{12})ky] + \beta_1[L_{11}+L_{12}+(L_{11}-L_{12})ky]\big]e^{ky}\cos(kx), \\ \varepsilon_{yy}^{(1)} &= \big[\alpha_1[2L_{12} + (L_{12}-L_{11})ky] + \beta_1[L_{12}+L_{11}+(L_{12}-L_{11})ky]\big]e^{ky}\cos(kx), \\ \varepsilon_{xy}^{(1)} &= L_{33}\big[\alpha_1(1+ky) + \beta_1 ky\big]e^{ky}\sin(kx). \end{aligned} \tag{4.24}$$

Further, by (4.19) the boundary traction on the nominal surface ∂B^0 is given by

$$\mathbf{p}^{(2)} = -h_0\partial_y(\mathbf{C}\nabla\mathbf{u}^{(1)})\mathbf{e}_2 + h_{0x}(\mathbf{C}\nabla\mathbf{u}^{(1)})\mathbf{e}_1 + \frac{1}{2}h_{0x}^2(\mathbf{C}\nabla\mathbf{u}^{(0)})\mathbf{e}_2 - h_{0xx}h_{0x}\sigma_{ss}^0\mathbf{e}_1, \tag{4.25}$$

where all derivatives are evaluated at $y = 0$. Below we evaluate the right hand side of the above equation term by term. First, by (4.23) we have that on ∂B^0 (i.e., $y = 0$),

$$\big[\sigma_{xx,y}^{(1)},\ \sigma_{yy,y}^{(1)},\ \sigma_{xy,y}^{(1)}\big] = \big[(3\alpha_1 + 2\beta_1)k\cos(kx),\ -\alpha_1 k\cos(kx),\ (2\alpha_1 + 2\beta_1)k\sin(kx)\big]. \tag{4.26}$$

Therefore,

$$\begin{aligned} &-h_0\partial_y(\mathbf{C}\nabla\mathbf{u}^{(1)})\mathbf{e}_2 = -(2\alpha_1 + 2\beta_1)k\sin(kx)\cos(kx)\mathbf{e}_1 + \alpha_1 k\cos^2(kx)\mathbf{e}_2, \\ &h_{0x}(\mathbf{C}\nabla\mathbf{u}^{(1)})\mathbf{e}_1 = -(2\alpha_1 + \beta_1)k\cos(kx)\sin(kx)\mathbf{e}_1 - \alpha_1 k\sin^2(kx)\mathbf{e}_2, \\ &\frac{1}{2}h_{0x}^2(\mathbf{C}\nabla\mathbf{u}^{(0)})\mathbf{e}_2 = 0, \\ &-h_{0xx}h_{0x}\sigma_{ss}^0\mathbf{e}_1 = \beta_1 k\cos(kx)\sin(kx)\mathbf{e}_1, \end{aligned}$$

and hence

$$p_x^{(2)} = \alpha_2\sin(2kx), \qquad p_y^{(2)} = \beta_2\cos(2kx), \tag{4.27}$$

where $\alpha_2 = -(2\alpha_1 + \beta_1)k = 2k^2\varepsilon_{xx}^{\infty}/L_{11} + k^3\tau^0$ and $\beta_2 = k\alpha_1 = -k^2\varepsilon_{xx}^{\infty}/L_{11}$. Comparing (4.27) with (4.22), we obtain the second order stress field, determined by the boundary value problem (3.3) and (3.4), by simply replacing (α_1, β_1) by (α_2, β_2) and k by $2k$:

$$\begin{aligned} \sigma_{xx}^{(2)} &= \big[\alpha_2(2+2ky) + \beta_2(1+2ky)\big]e^{2ky}\cos(2kx), \\ \sigma_{yy}^{(2)} &= -\big[\alpha_2 2ky + \beta_2(2ky-1)\big]e^{2ky}\cos(2kx), \\ \sigma_{xy}^{(2)} &= \big[\alpha_2(1+2ky) + \beta_2 2ky\big]e^{2ky}\sin(2kx). \end{aligned} \tag{4.28}$$

The associated second-order strain field follows from the constitutive relation (4.1). In particular,

$$\varepsilon_{xx}^{(2)} = \big[\alpha_2[2L_{11} + 2ky(L_{11}-L_{12})] + \beta_2[L_{11}+L_{12}+2ky(L_{11}-L_{12})]\big]e^{2ky}\cos(2kx). \tag{4.29}$$

To calculate surface elastic energy, we evaluate the surface strain on ∂B and express it in the frame $\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3 = \mathbf{e}_z\}$. By (4.6), (4.7) and (4.3), direct calculations show

$$\nabla \mathbf{u}\Big|_{y=h(x)} = \varepsilon_{ss}\mathbf{t}_1 \otimes \mathbf{t}_1 + \cdots, \tag{4.30}$$

and

$$\begin{aligned}\varepsilon_{ss} &= \mathbf{t}_1 \cdot \mathbf{H}\mathbf{t}_1 = (\mathbf{N}^T\mathbf{H}\mathbf{N})_{11} \\ &= [\mathbf{H}^0 + \delta(\mathbf{H}^1 + \mathbf{W}\mathbf{H}^0 + \mathbf{H}^0\mathbf{W}^T) + \delta^2(\mathbf{H}^2 + \mathbf{W}\mathbf{H}^1 + \mathbf{H}^1\mathbf{W}^T - h_{0x}^2\mathbf{H}^0)]_{11} + o(\delta^2) \\ &=: \varepsilon_{ss}^{(0)} + \delta\varepsilon_{ss}^{(1)} + \delta^2\varepsilon_{ss}^{(2)} + o(\delta^2),\end{aligned} \tag{4.31}$$

where $\mathbf{H}^k$ shall be evaluated at $y = 0$ and, by (4.17), (4.24), (4.29), we have

$$\begin{aligned}&\varepsilon_{ss}^{(0)} = H_{11}^0 = \varepsilon_{xx}^\infty, \qquad \varepsilon_{ss}^{(1)} = H_{11}^1 = \big[\alpha_1 2L_{11} + \beta_1(L_{11} + L_{12})\big]\cos(kx), \\ &\varepsilon_{ss}^{(2)} = H_{11}^2 + h_{0x}(H_{12}^1 + H_{21}^1) - h_{0x}^2 H_{11}^0 \\ &\quad = \big[\alpha_2 2L_{11} + \beta_2(L_{11} + L_{12})\big]\cos(2kx) \\ &\qquad +[(3L_{11} - L_{12})\alpha_1 + 2L_{11}\beta_1]k\cos^2(kx) - (2L_{33}k\alpha_1 + k^2\varepsilon_{xx}^\infty)\sin^2(kx).\end{aligned} \tag{4.32}$$

As discussed in §3 (cf., (3.5)-(3.7)), our homogenization scheme requires calculation of the total energy under the application of a far-field uniform strain. Since the domain is infinite, in the state of plane strain or plane stress, and invariant under a translation of wavelength $\lambda = 2\pi/k$ in $\mathbf{e}_x$-direction, we shall restrict our integration domain to the semi-infinite tube-like domain $T = (0, \lambda) \times (-\infty, h(x))$ for the half-space with rough surface, and $T^0 = (0, \lambda) \times (-\infty, 0)$ for the nominal flat half-space. By our solutions up to the second-order, i.e., (4.16), (4.23), (4.28) and (4.31) we now evaluate the actual total energy (cf., (3.5))

$$\begin{aligned}E^{\text{act}} &= \frac{1}{2\lambda}\int_T [\nabla\mathbf{u} \cdot \mathbf{C}\nabla\mathbf{u} - \nabla\mathbf{u}^{(0)} \cdot \mathbf{C}\nabla\mathbf{u}^{(0)}] + \frac{1}{\lambda}\int_{S_T}\Big[\frac{1}{2}\nabla\mathbf{u} \cdot \mathbf{C}_s\nabla\mathbf{u} + \nabla\mathbf{u} \cdot \mathbf{S}_s^0 + \gamma\Big] \\ &=: I + J,\end{aligned} \tag{4.33}$$

where $S_T = \{(x, y) : y = h(x), x \in (0, \lambda)\}$ is the rough surface on the semi-infinite tube T.

Due to the degeneracy of surface stiffness tensor (cf., (2.4)) and the assumption of plane strain or plane stress, we find that for any strain tensor $\mathbf{H}$ with surface strain $\epsilon = \mathbf{t}_1 \cdot \mathbf{H}\mathbf{t}_1$ within xy-plane,

$$\mathbf{H} \cdot \mathbf{C}_s\mathbf{H} = k^s\epsilon^2, \tag{4.34}$$

where

$$k^s = 2\mu^s + \lambda^s \ \ \text{(plane strain)} \quad \text{or} \quad 2\mu_s(1 + \nu^2) + \lambda_s(1 - \nu)^2 \ \ \text{(plane stress)}. \tag{4.35}$$

Further, it will be convenient to introduce vector fields $\mathbf{s}^{(i)} = [\sigma_{xx}^{(i)}, \sigma_{yy}^{(i)}, \sqrt{2}\sigma_{xy}^{(i)}]$ formed by components of the ith-order stress fields ($i = 1, 2$). Direct calculation verifies

$$\nabla\mathbf{u}^{(i)} \cdot \mathbf{C}\nabla\mathbf{u}^{(i)} = \mathbf{s}^{(i)} \cdot \mathbf{L}\mathbf{s}^{(i)} = \mathbf{L} \cdot (\mathbf{s}^{(i)} \otimes \mathbf{s}^{(i)}). \tag{4.36}$$

Then, the right hand side of (4.33) can be rewritten as

$$
\begin{aligned}
&I = \delta I_1 + \delta^2 I_2 + o(\delta^2), \qquad\qquad J = J_0 + \delta J_1 + \delta^2 J_2 + o(\delta^2),\\
&I_1 = \frac{1}{\lambda}\int_T \nabla \mathbf{u}^{(1)} \cdot \mathbf{C}\nabla \mathbf{u}^{(0)},\\
&I_2 = \frac{1}{\lambda}\int_T \big[\nabla \mathbf{u}^{(2)} \cdot \mathbf{C}\nabla \mathbf{u}^{(0)} + \frac{1}{2}\nabla \mathbf{u}^{(1)} \cdot \mathbf{C}\nabla \mathbf{u}^{(1)}\big],\\
&J_0 = \frac{1}{\lambda}\int_{S_T} [\frac{1}{2}k^s(\varepsilon_{ss}^{(0)})^2 + \tau^0\varepsilon_{ss}^{(0)} + \gamma], \qquad J_1 = \frac{1}{\lambda}\int_{S_T} \varepsilon_{ss}^{(1)}(k^s\varepsilon_{ss}^{(0)} + \tau^0),\\
&J_2 = \frac{1}{\lambda}\int_{S_T} \Big[\varepsilon_{ss}^{(2)}(k^s\varepsilon_{ss}^{(0)} + \tau^0) + \frac{1}{2}k^s(\varepsilon_{ss}^{(1)})^2\Big]
\end{aligned}
\tag{4.37}
$$

The above integrals can be evaluated term by term as follows. First, since the length of an infinitesimal segment on S_T is given by $ds = \Gamma(\delta, x)dx$ and $\Gamma(\delta, x) = \sqrt{1 + \delta^2 k^2 \sin^2 kx} \approx 1 + \frac{1}{2}\delta^2 k^2 \sin^2 kx$, we have

$$
J_0 = \frac{1}{\lambda}\int_0^\lambda [\frac{1}{2}k^s(\varepsilon_{ss}^{(0)})^2 + \tau^0\varepsilon_{ss}^{(0)} + \gamma]\Gamma(\delta, x) \approx [\frac{1}{2}k^s(\varepsilon_{xx}^\infty)^2 + \tau^0\varepsilon_{xx}^\infty + \gamma](1 + \frac{\delta^2 k^2}{4}). \tag{4.38}
$$

To evaluate I_1 and J_1, it is sufficient to compute terms up to the order of δ. By (B.1) we obtain

$$
\begin{aligned}
I_1 &= \frac{1}{\lambda}\int_0^\lambda \int_{-\infty}^{h(x)} \frac{\varepsilon_{xx}^\infty}{L_{11}}\varepsilon_{xx}^{(1)} dydx = \frac{\delta\varepsilon_{xx}^\infty}{2L_{11}}[2L_{11}\alpha_1 + \beta_1(L_{11} + L_{12})] + o(\delta)\\
&= \delta\Big[-\frac{k(\varepsilon_{xx}^\infty)^2}{L_{11}} - \frac{k^2(L_{11} + L_{12})\tau^0\varepsilon_{xx}^\infty}{2L_{11}}\Big] + o(\delta),\\
J_1 &= \frac{1}{\lambda}\int_0^\lambda \varepsilon_{ss}^{(1)}(k^s\varepsilon_{ss}^{(0)} + \tau^0)\Gamma(\delta, x) = o(\delta).
\end{aligned}
\tag{4.39}
$$

Finally, for I_2 and J_2 it is sufficient to calculate terms up to the order of 1. Since

$$
\frac{1}{\lambda}\int_T \nabla \mathbf{u}^{(2)} \cdot \mathbf{C}\nabla \mathbf{u}^{(0)} = \frac{1}{\lambda}\int_0^\lambda \int_{-\infty}^0 \nabla \mathbf{u}^{(2)} \cdot \mathbf{C}\nabla \mathbf{u}^{(0)} + o(1) = o(1), \tag{4.40}
$$

by (B.2) we find

$$
\begin{aligned}
I_2 &= \frac{1}{\lambda}\int_T \frac{1}{2}\nabla \mathbf{u}^{(1)} \cdot \mathbf{C}\nabla \mathbf{u}^{(1)} + o(1) = \frac{1}{\lambda}\int_T \frac{1}{2}\mathbf{L} \cdot (\mathbf{s}^{(i)} \otimes \mathbf{s}^{(i)}) + o(1) = \frac{1}{2}\mathbf{L} \cdot \mathbf{M}^*(k) + o(1),\\
J_2 &= \frac{1}{2}k^2[\varepsilon_{xx}^\infty(\frac{2L_{33} + L_{12}}{L_{11}} - 4) - 2L_{11}\tau^0 k](k^s\varepsilon_{xx}^\infty + \tau^0)\\
&\qquad + \frac{k^2k^s}{4}[2\varepsilon_{xx}^\infty + k\tau^0(L_{11} + L_{12})]^2 + o(1).
\end{aligned}
\tag{4.41}
$$

where

$$
\begin{aligned}
\mathbf{M}^*(k) &:= \frac{1}{\lambda}\int_0^\lambda \int_{-\infty}^{h(x)} \mathbf{s}^{(1)} \otimes \mathbf{s}^{(1)} dydx \\
&= \frac{k}{4}\begin{bmatrix}
\frac{5(\varepsilon_{xx}^\infty)^2}{2L_{11}^2} + \frac{2k\tau^0(\varepsilon_{xx}^\infty)}{L_{11}} + \frac{k^2(\tau^0)^2}{2} & \frac{(\varepsilon_{xx}^\infty)^2}{2L_{11}^2} + \frac{2k\tau^0(\varepsilon_{xx}^\infty)}{L_{11}} + \frac{k^2(\tau^0)^2}{2} & \\
\frac{(\varepsilon_{xx}^\infty)^2}{2L_{11}^2} + \frac{2k\tau^0(\varepsilon_{xx}^\infty)}{L_{11}} + \frac{k^2(\tau^0)^2}{2} & \frac{(\varepsilon_{xx}^\infty)^2}{2L_{11}^2} + \frac{2k\tau^0(\varepsilon_{xx}^\infty)}{L_{11}} + \frac{5k^2(\tau^0)^2}{2} & \\
 & & \frac{(\varepsilon_{xx}^\infty)^2}{L_{11}^2} + k^2(\tau^0)^2
\end{bmatrix},
\end{aligned}
\tag{4.42}
$$

and other components of $\mathbf{M}^*$ are not computed since they do not contribute in the product $\mathbf{L}\cdot\mathbf{M}^*$.

By (3.6) and (3.7), we define the effective properties of the nominal flat surface as

$$E^{\mathrm{act}} = E^{\mathrm{eff}} =: \frac{1}{\lambda}\int_0^\lambda \Big[\frac{1}{2}(k^s)^{\mathrm{eff}}(\varepsilon_{xx}^{(0)})^2 + \varepsilon_{xx}^{(0)}(\tau^0)^{\mathrm{eff}} + \gamma^{\mathrm{eff}}\Big]. \tag{4.43}$$

By (4.33), (4.38) and (4.43), we find the effective properties of the nominal flat surface to be

$$\begin{aligned}
\gamma^{\mathrm{eff}} &= \gamma + \delta^2\Big[k^2\frac{\gamma}{4} + k^3\frac{(\tau^0)^2}{8}(-5L_{11}+L_{12}+L_{33}) + k^4\frac{k^s(\tau^0)^2}{4}(L_{11}+L_{12})^2\Big],\\
(\tau^0)^{\mathrm{eff}} &= \tau^0 + \delta^2\tau^0\Big[k^2(-\frac{7}{4}+\frac{L_{33}}{L_{11}}+\frac{L_{12}}{2L_{11}}) + k^3k^sL_{12}\Big],\\
(k^s)^{\mathrm{eff}} &= k^s + \delta^2\Big[k(-\frac{5}{4L_{11}}+\frac{L_{12}+L_{33}}{4L_{11}^2}) + k^2k^s(-\frac{7}{4}+\frac{2L_{33}+L_{12}}{L_{11}})\Big].
\end{aligned} \tag{4.44}$$

By the assumption (4.13), the last terms in the above equations can be neglected compared to the remaining ones inside the bracket. Inserting (4.2) into the above equations, we obtain the effective properties in terms of the familiar isotropic elastic constants:

- plane strain ($\mu = E/2(1+\nu)$ is the shear modulus):

$$\begin{aligned}
\gamma^{\mathrm{eff}} &= \gamma + \delta^2\Big[k^2\frac{\gamma}{4} - k^3(\tau^0)^2\frac{(1-\nu)}{4\mu}\Big],\\
(\tau^0)^{\mathrm{eff}} &= \tau^0\Big[1-\delta^2k^2\frac{3-5\nu}{4(1-\nu)}\Big],\\
(k^s)^{\mathrm{eff}} &= k^s - \delta^2k\frac{2\mu}{1-\nu};
\end{aligned} \tag{4.45}$$

- plane stress:

$$\begin{aligned}
\gamma^{\mathrm{eff}} &= \gamma + \delta^2\Big[k^2\frac{\gamma}{4} - k^3(\tau^0)^2\frac{1}{2E}\Big],\\
(\tau^0)^{\mathrm{eff}} &= \tau^0\Big[1-\delta^2k^2\frac{3-2\nu}{4}\Big],\\
(k^s)^{\mathrm{eff}} &= k^s - \delta^2kE.
\end{aligned} \tag{4.46}$$

We remark that the above solutions for a particular loading condition, i.e., a uniaxial remote stress $\sigma^\infty\mathbf{e}_1\otimes\mathbf{e}_1$ at infinity, are insufficient to determine the full effective surface elasticity tensor $\mathbf{C}_s^{\mathrm{eff}}$ or effective residual surface stress tensor $(\mathbf{S}_s^0)^{\mathrm{eff}}$ defined by (3.7). By (4.21), we identify the zeroth order surface strain tensor as given by $\varepsilon_{xx}^{(0)}\hat{\mathbf{H}}$, and in the basis $\{\mathbf{t}_1,\mathbf{e}_z\}$ the tensor $\hat{\mathbf{H}}$ is given by

$$\hat{\mathbf{H}} = \begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\ \text{(plane strain)} \qquad \text{or} \qquad \begin{bmatrix}1 & 0\\ 0 & -\nu\end{bmatrix}\ \text{(plane stress)}.$$

By (3.7), (4.21) and (4.43) we identify the following relations

$$(k^s)^{\mathrm{eff}} = \hat{\mathbf{H}}\cdot\mathbf{C}_s^{\mathrm{eff}}\hat{\mathbf{H}}, \qquad (\tau^0)^{\mathrm{eff}} = (\mathbf{S}_s^0)^{\mathrm{eff}}\cdot\hat{\mathbf{H}}.$$

Finally, it is worthwhile noticing that the effective properties are in fact independent of the second order solution which is by no means obvious *a priori*.

4.3 General roughness

We now consider a general roughness profile. Assume $h(x) = \delta h_0(x)$ with $h_0(x) \sim 1$, $\delta << 1$. By choosing a large enough $\Lambda > 0$, we may without loss of generality assume $h_0(x)$ is even and a periodic function with period Λ. In another word, the roughness is statistically invariant over a lengthscale of Λ. By Fourier analysis we have ($\mathcal{K}_+ = \frac{2\pi}{\Lambda}\{1, 2, \cdots\}$)

$$h_0(x) = \sum_{m\in\mathcal{K}_+} \hat{h}_0(m)\cos(mx), \qquad \hat{h}_0(m) = \frac{2}{\Lambda}\int_0^\Lambda h_0(x)\cos(mx)dx. \tag{4.47}$$

It will be useful to introduce constants which are properties of the roughness profile $h_0(x)$:

$$\Omega^{(i)} = \sum_{m\in\mathcal{K}_+} m^i|\hat{h}_0(m)|^2. \tag{4.48}$$

Applying the same procedure in the previous section for each mode $m \in \mathcal{K}_+$, we obtain the perturbed stress fields as in (4.23) and (4.28) with k being replaced by m, and

$$\begin{aligned}
\alpha_1 &= -\hat{h}_0(m)m\frac{\epsilon_{xx}^\infty}{L_{11}}, \qquad & \beta_1 &= -\hat{h}_0(m)m^2\tau^0,\\
\alpha_2 &= -(2\alpha_1+\beta_1)m, \qquad & \beta_2 &= m\alpha_1.
\end{aligned}$$

To evaluate the actual elastic energy, from (4.33)-(4.41) and Parseval's theorem we observe that different modes do not interact in the sense that the integrals defined in (4.37) are simply a summation of all modes:

$$\begin{aligned}
I_1 &= \delta\sum_{m\in\mathcal{K}_+}\Big[-|\hat{h}_0(m)|^2\frac{m(\varepsilon_{xx}^\infty)^2}{L_{11}} - |\hat{h}_0(m)|^2\frac{m^2(L_{11}+L_{12})\tau^0}{2L_{11}}\varepsilon_{xx}^\infty\Big] + o(\delta),\\
I_2 &= \sum_{m\in\mathcal{K}_+}\frac{1}{2}|\hat{h}_0(m)|^2\mathbf{L}\cdot\mathbf{M}^*(m) + o(1),\\
J_0 &= \sum_{m\in\mathcal{K}_+}[\frac{1}{2}k^s(\varepsilon_{xx}^\infty)^2 + \tau^0\varepsilon_{xx}^\infty + \gamma](1 + \frac{\delta^2m^2}{4}|\hat{h}_0(m)|^2), \qquad J_1 = o(\delta),\\
J_2 &= \sum_{m\in\mathcal{K}_+}\Big\{\frac{1}{2}|\hat{h}_0(m)|^2m^2[\varepsilon_{xx}^\infty(\frac{2L_{33}+L_{12}}{L_{11}} - 4) - 2L_{11}\tau^0m](k^s\varepsilon_{xx}^\infty + \tau^0)\\
&\qquad + |\hat{h}_0(m)|^2\frac{m^2k^s}{4}[2\varepsilon_{xx}^\infty + m\tau^0(L_{11}+L_{12})]^2\Big\} + o(1).
\end{aligned}$$

Therefore, the effective properties of the nominal flat surface for a general rough surface are given by

$$\begin{aligned}
\gamma^{\text{eff}} &= \gamma + \delta^2\Big[\Omega^{(2)}\frac{\gamma}{4} + \Omega^{(3)}\frac{(\tau^0)^2}{8}(-5L_{11}+L_{12}+L_{33})\Big],\\
(\tau^0)^{\text{eff}} &= \tau^0 + \delta^2\tau^0\Big[\Omega^{(2)}(-\frac{7}{4} + \frac{L_{33}}{L_{11}} + \frac{L_{12}}{2L_{11}})\Big],\\
(k^s)^{\text{eff}} &= k^s + \delta^2\Omega^{(1)}(-\frac{5}{4L_{11}} + \frac{L_{12}+L_{33}}{4L_{11}^2}).
\end{aligned} \tag{4.49}$$

4.4 Random roughness

We now consider an ensemble of random surfaces. Assume that

$$\langle h_0(x)\rangle = 0, \qquad \langle h_0(x_1)h_0(x_2)\rangle = \kappa(|x_1 - x_2|) \qquad \forall\, x,\, x_1,\, x_2 \in \mathbb{R}, \tag{4.50}$$

where $\langle\ \rangle$ denotes the ensemble average, and $\kappa : \mathbb{R} \to \mathbb{R}$ is referred to as the *autocorrelation function*. Typically, the autocorrelation function $\kappa(t)$ is even, smooth and negligible if $t > l_c$, where l_c is the correlation length. The autocorrelation function and correlation length are statistical properties of roughness which are experimentally measurable. Without loss of generality, we further assume every realization of random roughness $h_0(x)$ is even and periodic with period $\Lambda >> l_c$. To find the ensemble average of the effective properties, by (4.49) we need to evaluate $\langle\Omega^{(i)}\rangle$ for $i = 1, 2, 3$. To this end, we introduce the *spectral density of fluctuation* $S(k)$ defined by

$$S(k)\triangle k = \sum_{k<m<k+\triangle k} \langle|\hat{h}_0(m)|^2\rangle. \tag{4.51}$$

By *Wiener-Khinchin theorem* (Van Kampen, 2007; p. 59), in the limit $\Lambda \to +\infty$ we have (cf., Appendix C)

$$S(m) = \frac{2}{\pi}\int_{\mathbb{R}} \kappa(t)\exp(-imt)dt = \frac{2}{\pi}\hat{\kappa}(m). \tag{4.52}$$

where $\hat{\kappa}(m) = \int_{\mathbb{R}} \kappa(t)\exp(-imt)dt$ is the Fourier transformation of $\kappa(t)$. Therefore, by (4.51) the moments $\Omega^{(i)}$ defined by (4.48) are given by

$$\Omega^{(j)} = \int_0^\infty m^j S(m)dm = \frac{2}{\pi}\int_0^\infty m^j \hat{\kappa}(m)dm. \tag{4.53}$$

By the inversion theorem, $\kappa^{(j)}(0) = \frac{1}{2\pi}\int_{\mathbb{R}}(im)^j\hat{\kappa}(m)dm$, and hence for even integer $2j$,

$$\frac{2}{\pi}\int_0^\infty m^{2j}\hat{\kappa}(m)dm = \frac{1}{\pi}\int_{\mathbb{R}} m^{2j}\hat{\kappa}(m)dm = (-1)^j 2\kappa^{(2j)}(0).$$

For an odd integer $2j+1$, a simple formula for $\Omega^{(2j+1)}$ as above is not available; one has to specify the autocorrelation function $\kappa(t)$ and compute it by (4.53).

As an example, assume the autocorrelation function is a Gaussian function

$$\kappa(t) = \exp(-\frac{t^2}{2l_c^2}),$$

where l_c can be identified as the correlation length. By definition the above equation implies that the standard deviation of roughness $\sqrt{\langle h^2(x)\rangle} = \delta\sqrt{\langle h_0^2(x)\rangle} = \delta\sqrt{\kappa(0)} = \delta$. Then the Fourier transformation of $\kappa(t)$ is given by

$$\hat{\kappa}(m) = l_c\sqrt{2\pi}\exp(-\frac{l_c^2 m^2}{2}),$$

and hence

$$\Omega^{(1)} = \frac{2}{l_c}\sqrt{\frac{2}{\pi}}, \qquad \Omega^{(2)} = \frac{2}{l_c^2}, \qquad \Omega^{(3)} = \frac{4}{l_c^3}\sqrt{\frac{2}{\pi}}.$$

Inserting the above equation into (4.49) and in terms of the familiar elastic constants, the effective surface properties are given by ($\eta = \delta/l_c$)

• plane strain:

$$\begin{aligned}
\gamma^{\text{eff}} &= \gamma + \eta^2\Big[\frac{\gamma}{2} - (\tau^0)^2\frac{(1-\nu)}{\mu l_c}\sqrt{\frac{2}{\pi}}\Big],\\
(\tau^0)^{\text{eff}} &= \tau^0\Big[1 - \eta^2\frac{3-5\nu}{2(1-\nu)}\Big],\\
(k^s)^{\text{eff}} &= k^s - \eta^2\frac{4\mu l_c}{1-\nu}\sqrt{\frac{2}{\pi}};
\end{aligned} \tag{4.54}$$

• plane stress:

$$\begin{aligned}
\gamma^{\text{eff}} &= \gamma + \eta^2\Big[\frac{\gamma}{2} - (\tau^0)^2\frac{2}{El_c}\sqrt{\frac{2}{\pi}}\Big],\\
(\tau^0)^{\text{eff}} &= \tau^0\Big[1 - \eta^2\frac{3-2\nu}{2}\Big],\\
(k^s)^{\text{eff}} &= k^s - \eta^2 2El_c\sqrt{\frac{2}{\pi}}.
\end{aligned} \tag{4.55}$$

5 Discussion, Atomistic Validation and Applications

We can use the simple expressions we have derived to make some assessments on the effect of roughness on the surface properties. We take Copper as an example, with Young's modulus E of 115 GPa, Poisson's ratio ν of 0.34, surface stress $\tau^0 \approx 1.04$N/m and surface elastic constant $k^s \approx -3.16$N/m of the (001) crystal face (Shenoy, 2005). If we consider sinusoidal roughness with $\delta k = 0.2$ and wave length λ around $10nm$, then the wave number $k = \frac{2\pi}{\lambda} \sim \frac{2\pi}{10^{-8}} = 6.28 \times 10^8\text{m}^{-1}$, and by (4.45) and (4.46) we have (for plane stress case):

$$(\gamma)^{\text{eff}} = 1.01\gamma, \qquad (\tau^0)^{\text{eff}} = 0.98\tau^0 \qquad (k^s)^{\text{eff}} = -10.485N/m. \tag{5.1}$$

So $(\tau^0)^{\text{eff}}$ for this rough surface is barely 2 percent less than the pristine value, τ^0. However, we observe a dramatic change in $(k^s)^{\text{eff}}$ from the flat surface value of $-3.16N/m$! Therefore, we can conclude that while residual surface stress is hardly affected by the roughness, the surface elastic parameters can change appreciably. It should be noted here that surface roughness can even cause a change of sign in surface elastic constants depending on the extent of the roughness. Finally, as evident from the expressions for the both the periodic and random roughness case, even if the bare surface possesses zero surface elasticity i.e. $k^s \approx 0$ roughness will "create" surface elasticity i.e. effective value of k^s will be non-zero.

Our theoretical predictions are, qualitatively, consistent with atomistic simulations we conducted on Silver. The sample geometry is shown in Figure (3). Further details of the atomistic simulations may be found in Mohammadi and Sharma (2012).

For the Silver cantilever nano-beam, we chose roughness with 0.215 nm amplitude and 1.636 nm wavelength. The bare values of surface stress and surface elastic constants are, respectively, 0.023 and -0.168 eV/A^2. We find $(\tau^0)^{\text{eff}}$ to be 0.01895 eV/A^2 from atomistics while our theoretical calculations predict 0.0225. On the other hand, k^s undergoes a larger change—atomistics predict -0.506 eV/A^2 qualitatively consistent with our theoretical prediction: -0.367 eV/A^2. Considering

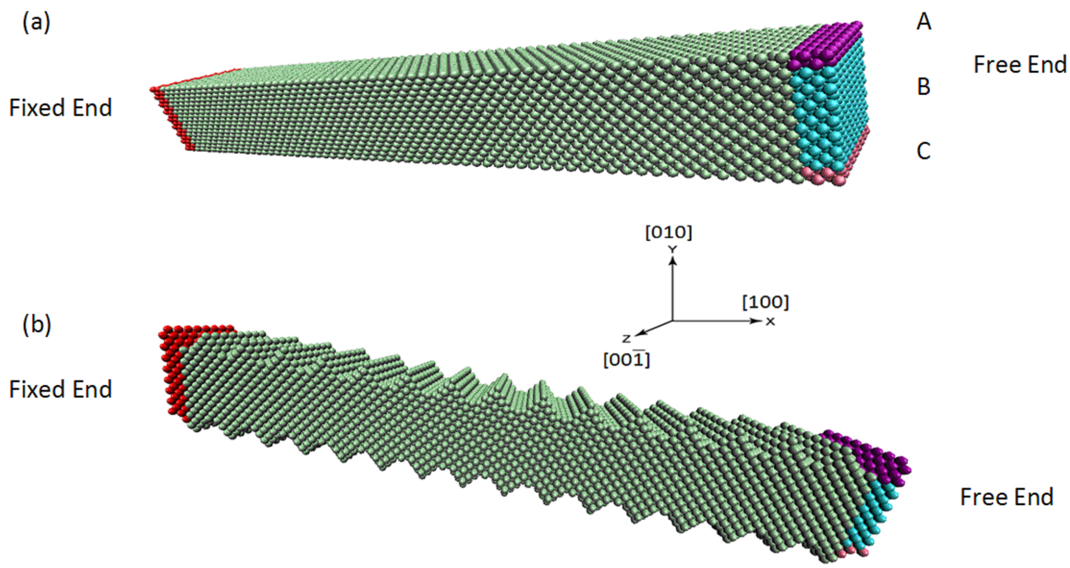

Figure 3: Atomistic calculations to extract the effect of roughness on surface elasticity (Mohammadi and Sharma, 2012)

that ours is a perturbation approach and the other assumptions we have made (e.g. isotropy), only a qualitative match can be expected in comparison with atomistics.

Weissmuller and Duan (2008) have shown that the response of the curvature of cantilevers to changes in their surface stress in the presence of the surface roughness is different from nominally planar surfaces. Considering surface residual stress for cantilevers, they concluded that deliberate structuring of the surface allows the magnitude and even its sign to be tuned. They have concluded that bending of the substrate is controlled by changes in in-plane component of the surface-induced stress, T only. Their calculation shows that T for the isotropic solid with a nearly planar surface $\theta^2 \ll 1$ (assuming isotropy) is equal to

$$T = \frac{\langle f \rangle_s}{h^1}\Big(1 - \frac{v^1}{1-v^1}\langle\theta^2\rangle\Big), \tag{5.2}$$

where f is surface residual stress and v^1 is the Poisson's ratio. In their calculations, they assumed that f depends on the surface orientation but this assumption does not have any contribution in creating the $(1 - \frac{v^1}{1-v^1}\langle\theta^2\rangle)$ term that shows that the apparent action of f will be reduced by a geometric effect that scales with the root-mean-square of θ. We note here that for sinusoidal roughness $\langle\theta^2\rangle$ is $\delta k/2$. Their model is different than ours and accordingly we don't make any further comparisons beyond noting that both our works are predicated on the "small roughness" assumption and that physical conclusions shall be used with caution when this assumption is violated.

Nanofabricated cantilever structures have been demonstrated to be extremely versatile sensors and have potential applications in physical, chemical, and biological sciences. Adsorption on surface of such a sensor may induce mass, damping, and stress changes of the cantilever response. One cantilever sensor technique is to monitor changes in the cantilever resonance frequency. The effect of surface stress on the resonance frequency of a cantilever have been modeled analytically by Lu et al. (2005) by incorporating strain-dependent surface stress terms into the equations of motion.

Consider a cantilever used as a sensor. The experimental quantity measured is the surface stress difference, $\triangle\sigma^s = \sigma_u^s - \sigma_l^s$, where σ_u^s and σ_l^s are the surface stresses on the upper and the lower surfaces, respectively. In the isotropic case, the surface stresses may be written as

$$\sigma_u^s = \tau_u^0 + k_u^s(\varepsilon^{ss})_u \text{ and } \sigma_\mathrm{l}^\mathrm{s} = \tau_\mathrm{l}^0 + \mathrm{k}_\mathrm{l}^\mathrm{s}(\varepsilon^{\mathrm{ss}})_\mathrm{l}, \tag{5.3}$$

where τ^0 is the strain-independent surface stress, k_s is the surface elastic modulus, ε_{ss} is the surface strain measured from the pre-stressed configuration, and the subscripts u and l always refer to the upper and lower surface, respectively. The surface stress difference can be written as

$$\triangle\sigma^s = \triangle\sigma^0 - \triangle\sigma^l, \tag{5.4}$$

with $\triangle\sigma^0 = \tau_u^0 - \tau_l^0$ and $\triangle\sigma^l = k_u^s(\varepsilon_{ss})_u - k_l^s(\varepsilon_{ss})_l$. While the strain-independent part of the surface stress, $\triangle\sigma^0$ can have an impact on the resonance frequency (in a nonlinear setting), it is expected to be small. The strain-dependent part (i.e. surface elasticity) definitely will change the resonance frequency and can be expressed as

$$Q \equiv \frac{(\omega_s)^2 - (\omega_0)^2}{(\omega_0)^2} = 3\frac{k_u^s + k_l^s}{Eh}, \tag{5.5}$$

where ω_0 is the fundamental resonance frequency without considering surface elasticity, ω_s is the resonance frequency with surface stresses acting, h is the thickness and E is Young's modulus. Liu and Rajapakse (2010) have also derived a similar expression

To compare the change in resonance frequency of cantilevers with rough surfaces, we consider a beam that has a sinusoidal rough surface on top and flat surface on the bottom. We have

$$k_u^s = (k^s)^{\mathrm{eff}} = k^s - \delta^2 kE \tag{5.6}$$

for top surface and $k_l^s = k^s$ for the lower surface. Then the change in resonance frequency can be obtained as

$$Q_{rough} = \frac{3}{Eh}\left(2k^s - \delta^2 kE\right) \tag{5.7}$$

Compared to a cantilever with upper and lower flat surface with resonance frequency

$$Q = \frac{3}{Eh}\left(2k^s\right) \tag{5.8}$$

We stress here that this calculation is approximate and intended to simply demonstrate the use of our results. A rigorous calculation may yield additional terms if roughness is directly modeled in calculation of the frequency shift as opposed to using homogenized effective properties. Keeping this caveat in mind, we can infer that the frequency shift will decrease significantly or even, in some cases, change sign. For instance, in case of copper (001) crystal face (Shenoy, 2005), if we consider a sinusoidal roughness with $ak = 0.2$ and wave length of 10 nm on the top surface of the cantilever, the change of resonance frequency can be calculated to be: $Q_{rough} = \frac{3}{Eh}(-13.64)$ from its value of $Q = \frac{3}{Eh}(-6.32)$. So quantitatively, the square of resonance frequency is shifted by nearly a factor of 2.

As another example, we consider aluminum with Young's modulus E of 70 GPa, Poisson's ratio v of 0.35, $\tau^0 \approx 0.91$ N/m and$k^s \approx 4.53$ N/m for the (111) crystal face (Shenoy, 2005). Then the result for the rough case is $\frac{3}{Eh}(5.87)$ as opposed to the flat case of $\frac{3}{Eh}(9.06)$.

In summary, we have presented simple expressions for the homogenized surface stress and surface elasticity for both randomly and periodically rough surfaces. Residual surface stress does not appear to be significantly affected by the presence of roughness although we do notice a dramatic change in the surface elastic modulus. The latter for example, as we demonstrated through simple illustrative quantitative examples, should have significant impact on the way sensing data based on surface effects is interpreted. We finally note an interesting observation that even if the bare surface has a zero surface elasticity modulus, roughness will endow it with one.

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Appendix A: Elasticity solution to two-dimensional isotropic half-space

Here we recall the classic solution to the elasticity problem of a two dimensional isotropic flat half-space $B^0 = \{(x, y) : y < 0\}$ subject to an applied traction $\mathbf{p} = (p_x,\ p_y)$ on $\partial B^0 = \{(x, y) : y = 0\}$. Let

$$(\hat{p}_x(m),\ \hat{p}_y(m)) = \int_{\mathbb{R}} (p_x(x),\ p_y(x)) e^{-imx} dx$$

be their Fourier transformations. Then the solutions to the stress and stain fields are given by (Asaro and Lubarda, 2006, pp. 229-232)

$$\begin{aligned}
\sigma_{xx}(x, y) &= \frac{1}{2\pi} \int_{\mathbb{R}} [\hat{p}_x(m)(-2\frac{|m|}{im} + imy) + \hat{p}_y(m)(1 + |m|y)] e^{imx+|m|y} dm, \\
\sigma_{yy}(x, y) &= \frac{1}{2\pi} \int_{\mathbb{R}} [-im\hat{p}_x(m)y + \hat{p}_y(m)(1 - |m|y)] e^{imx+|m|y} dm, \\
\sigma_{xy}(x, y) &= \frac{1}{2\pi} \int_{\mathbb{R}} [\hat{p}_x(m)(1 + |m|y) - im\hat{p}_y(m)y] e^{imx+|m|y} dm.
\end{aligned} \tag{A.1}$$

Appendix B: Evaluation of the selected integrals used in Section 4.2

First, we recall a few identities for $\eta << 1$ (which may be verified by Mathematica):

$$\begin{aligned}
&\frac{1}{2\pi} \int_0^{2\pi} \sin^2 \theta d\theta = \frac{1}{2}, \quad \int_{-\infty}^{h} y e^y dy = e^h(-1 + h), \quad \int_{-\infty}^{h} y^2 e^y dy = e^h(2 - h + h^2), \\
&\frac{1}{2\pi} \int_0^{2\pi} e^{\eta \cos\theta} \cos\theta d\theta = \frac{\eta}{2} + o(\eta), \quad \int_0^{2\pi} e^{\sin\theta} \cos\theta d\theta = 0, \\
&\int_0^{2\pi} e^{\eta\cos\theta}(-1 + \eta\cos\theta) \cos\theta d\theta = o(\eta).
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\frac{1}{\lambda} \int_0^{\lambda} \int_{-\infty}^{h(x)} k y e^{ky} \cos(kx) dy dx = \frac{1}{2\pi} \int_0^{\lambda} e^{\delta k \cos(kx)}(-1 + \delta k \cos(kx)) \cos(kx) dx = o(\delta), \\
&\frac{1}{\lambda} \int_0^{\lambda} \int_{-\infty}^{h(x)} e^{ky} \cos(kx) dy dx = \frac{1}{2\pi} \int_0^{\lambda} e^{\delta k \cos(kx)} \cos(kx) dx = \frac{\delta}{2} + o(\delta), \\
&\frac{1}{\lambda} \int_0^{\lambda} \int_{-\infty}^{h(x)} \varepsilon_{xx}^{(1)} dy dx = \frac{\delta}{2}[2L_{11}\alpha_1 + \beta_1(L_{11} + L_{12})] + o(\delta).
\end{aligned} \tag{B.1}$$

Further, we notice that for any constants A, B, C,

$$\frac{1}{\lambda}\int_0^\lambda \int_{-\infty}^{h(x)} (A + B(2ky) + C(2ky)^2)e^{2ky}\cos^2(kx)dydx = \frac{1}{4k}(A - B + 2C) + o(1).$$

Therefore,

$$\begin{aligned} &\frac{1}{\lambda}\int_0^\lambda \int_{-\infty}^{h(x)} \mathbf{s}^{(1)} \otimes \mathbf{s}^{(1)} dydx = \mathbf{M}^* \\ &\approx \frac{1}{4k}\begin{bmatrix} \alpha_1(2\alpha_1+\beta_1) + \frac{(\alpha_1+\beta_1)^2}{2} & \alpha_1\beta_1 + \frac{(\alpha_1+\beta_1)^2}{2} & \\ \alpha_1\beta_1 + \frac{(\alpha_1+\beta_1)^2}{2} & \beta_1(\alpha_1+2\beta_1) + \frac{(\alpha_1+\beta_1)^2}{2} & \\ & & -2\beta_1\alpha_1 + (\alpha_1+\beta_1)^2 \end{bmatrix}, \end{aligned} \tag{B.2}$$

where other components of $\mathbf{M}^*$ are not computed since they do not contribute to the product $\mathbf{L}\cdot\mathbf{M}^*$.

Appendix C: Wiener-Khinchin Theorem

We outline the argument for (4.52) as follows. First, we notice that

$$\begin{aligned} \langle|\hat{h}_0(m)|^2\rangle &= \frac{4}{\Lambda^2}\left\langle \int_0^\Lambda \int_0^\Lambda h_0(x_1)h_0(x_2)\exp(im(x_1-x_2))dx_1dx_2 \right\rangle \\ &= \frac{4}{\Lambda^2}\int_0^\Lambda \int_0^\Lambda \langle h_0(x_1)h_0(x_2)\rangle \exp(im(x_1-x_2))dx_1dx_2 \\ &= \frac{4}{\Lambda^2}\int_0^\Lambda \int_0^\Lambda \kappa(x_1-x_2)\exp(im(x_1-x_2))dx_1dx_2 \\ &= \frac{4}{\Lambda^2}\int_0^\Lambda dx_1 \int_{-x_1}^{\Lambda-x_1} \kappa(t)\exp(-imt)dt. \end{aligned}$$

Since $\kappa(t)$ is negligible if $t > l_c$, in the limit $\Lambda \to +\infty$ we have

$$\begin{aligned} \sum_{k<m<k+\Delta k} \langle|\hat{h}_0(m)|^2\rangle &= \sum_{k<m<k+\Delta k} \frac{2}{\pi\Lambda}\int_0^\Lambda dx_1 \frac{2\pi}{\Lambda}\int_{-x_1}^{\Lambda-x_1} \kappa(t)\exp(-imt)dt \\ &\to \frac{2}{\pi}\int_{\mathbb{R}} \kappa(t)\exp(-imt)dt = \frac{2}{\pi}\hat{\kappa}(m), \end{aligned}$$

which completes the proof of (4.52).

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