Journal of the Mechanics and Physics of Solids 61 (2013) 325–340

Contents lists available at SciVerse ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Surface energy, elasticity and the homogenization of rough surfaces

P. Mohammadi [a], L.P. Liu [c,d], P. Sharma [a,b,*], R.V. Kukta [e]

[a] Department of Mechanical Engineering, University of Houston, Houston, TX 77204, USA
[b] Department of Physics, University of Houston, Houston, TX 77204, USA
[c] Department of Mathematics, Rutgers University, NJ 08854, USA
[d] Department of Mechanical Aerospace Engineering, Rutgers University, NJ 08854, USA
[e] Department of Mechanical Engineering, Stony Brook University, Stony Brook, NY, USA

ARTICLE INFO

Article history:
Received 26 April 2011
Received in revised form
15 October 2012
Accepted 24 October 2012
Available online 6 November 2012

Keywords:
Surface energy
Roughness
Homogenization
Surface elasticity
Surface stress

ABSTRACT

The concept of surface energy is widely used to understand numerous aspects of material behavior: fracture, self-assembly, catalysis, void formation, microstructure evolution, and size-effect exhibited by nanostructures. 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 both nanostructures and bulk material where surfaces are involved in some form or fashion. 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

Surface atoms have different coordination numbers, mechanical, and chemical properties. These differences are manifested phenomenologically in that the various bulk properties such as elastic modulus, melting temperature, electromagnetic properties among 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 de 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

* Corresponding author at: Department of Mechanical Engineering, University of Houston, Houston, TX 77204, USA. Tel.: +1 713 743 4256.
E-mail address: psharma@uh.edu (P. Sharma).

0022-5096/$ - see front matter
http://dx.doi.org/10.1016/j.jmps.2012.10.010

line of works exists that are more materials oriented: Cahn (1989), Streitz et al. (1994), Weissmuller and Cahn (1997), Johnson (2000), Voorhees and Johnson (2004), and Cammarata (1994a,b) 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,b; 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), nano-particles, wires and films (Streitz et al., 1994; Diao et al., 2003, 2004a,b; Villain et al., 2004; Dingreville et al., 2005), sensing and vibration (Wang and Feng, 2007; Park and Klein, 2008; Park, 2009), and 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), and 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), and Schiavone and Ru (2009). The papers by Wang et al. (2010a,b) 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 be artificially tailored to obtain desired surface characteristics? These questions are at the heart of the present paper. 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. (2010a,b) 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, $\mathbf{u}:B\to\mathbb{R}^3$ be a vector field, and $\mathbf{T}:B\to\mathrm{Lin}(\mathbb{R}^3,\mathbb{R}^3):=\{\mathbf{M}:\mathbb{R}^3\to\mathbb{R}^3$ is linear$\}$ be a tensor field. Suppose that φ, $\mathbf{u}$, and $\mathbf{T}$

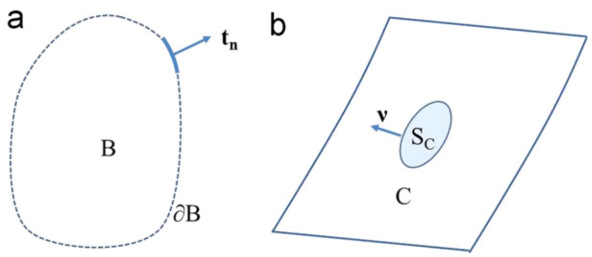

Fig. 1. (a) An elastic body $B\subset\mathbb{R}^3$ with surface ∂B and unit outward normal $\mathbf{t}_n$ and (b) the subsurface $S_C\subset\partial B$ enclosed by a simple contour C with unit outward normal $\boldsymbol{\nu}$ within the surface.