International Journal of Solids and Structures 96 (2016) 153–161

Contents lists available at ScienceDirect

International Journal of Solids and Structures

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

Surface effects in an elastic solid with nanosized surface asperities

M.A. Grekov*, S.A. Kostyrko

Department of Computational Methods in Continuum Mechanics, St. Petersburg State University, 7/9 Universitetskaya nab., St. Petersburg, 199034, Russia

ARTICLE INFO

Article history:
Received 4 November 2015
Revised 4 April 2016
Available online 8 June 2016

Keywords:
Surface asperities
Surface stress
Surface tension
Stress concentration
Size effect

ABSTRACT

The effects of surface elasticity and surface tension on the stress field near nanosized surface asperities having at least one dimension in the range 1–100 nm is investigated. The general two-dimensional problem for an isotropic stressed solid with an arbitrary roughened surface at the nanoscale is considered. The bulk material is idealized as an elastic semi-infinite continuum. In accordance with the Gurtin–Murdoch model, the surface is represented as a coherently bonded elastic membrane. The surface properties are characterized by the residual surface stress (surface tension) and the surface Lame constants, which differ from those of the bulk. The boundary conditions at the curved surface are described by the generalized Young–Laplace equation. Using a specific approach to the boundary perturbation technique, Goursat–Kolosov complex potentials, and Muskhelishvili representations, the boundary value problem is reduced to the solution of a hypersingular integral equation. Based on the first-order approximation, some numerical results in the case of a periodic shape of the surface and the analysis of the influence of surface stress, surface tension, the surface shape, and the size of the asperity on the hoop stress at the surface are presented. It is found that the surface tension alone produces a high level of stress concentration, much more than can be reduced by surface stress arising as a result of deformation. The stress formula obtained by Gao (1991) for sinusoidal surfaces at the macrolevel is extended to nanosized surface asperities.

1. Introduction

Many defects, such as vacancies, interstitials, dislocations, disclinations, crystal twins, nanoclusters, and microcracks, are located in a subsurface of a real material. This is one of the reasons that an initially smooth surface becomes roughened under a number of natural phenomena: heat, light, short-wavelength electromagnetic radiation, radioactive emissions, chemicals, mechanical stress, etc. (Medina and Hilderliter, 2014; Pronina, 2015; Sedova and Pronina, 2015). For instance, under mechanical loading, surface asperities with lateral sizes of about a hundred nanometers and vertical sizes about ten nanometers, that arise on mechanically and/or chemically polished Si(111) and Ge(111) surfaces of plates made from cylindrical mono-crystal products, has been addressed by Betechtin et al. (2003). The same formations of a wavy surface roughness in heteroepitaxial films have been observed by Ozkan et al. (1997). Various examples of nanostructured surfaces and surface effects are described by Rosei (2004) in a paper which extends and complements a previous review (Moriarty, 2001).

The principal aim of the present paper is to extend a complex variables based technique, applied previously to the analysis of elastic materials with macro asperities of a slightly curved surface (Grekov and Kostyrko, 2015; Grekov and Makarov, 2004; Vikulina et al., 2010) and interface (Grekov, 2004, 2011; Grekov and Kostyrko, 2013), to a problem involving surface nano_asperities similar to those observed by Ozkan et al. (1997) and Betechtin et al. (2003). We prove that this technique is an extremely powerful tool in the analysis of the elastic fields around nanosized surface asperities.

Surface asperities are the source of stress concentrations. Analyzing a sinusoidal surface perturbation of a stressed solid at the macrolevel, Gao (1991) has shown that even a slightly undulating surface can generate significant stress concentration that can induce fracture before the bulk stress reaches a critical level. Similar results have been analytically obtained for cycloid-shaped surfaces (Chiu and Gao, 1993), arbitrary weakly curved surfaces (Grekov and Kostyrko, 2015; Grekov and Makarov, 2004; Medina, 2015; Medina and Hilderliter, 2014; Vikulina et al., 2010), and interfaces (Grekov, 2004, 2011; Grekov and Kostyrko, 2013).

All of these solutions are suitable for the case of macroscale roughness when the effect of surface tension and surface elasticity on the stress state of the solid is negligible in comparison with the effect of the macroscopic bulk elastic behavior. At the same

* Corresponding author. Tel.: +79217480608.
E-mail addresses: magrekov@mail.ru (M.A. Grekov), sergey.kostyrko@gmail.com (S.A. Kostyrko).

http://dx.doi.org/10.1016/j.ijsolstr.2016.06.013
0020-7683/

time, it was observed by Wang et al. (2011) that the mechanics of nanosized structural elements, such as nanoparticles, nanowires, nanobeams, nanoplates, and nanoshels as well as heterogeneous materials containing nanoscale inhomogeneities deviates notably from general classical mechanics. Unlike bulk material elements, the nanostructures have elastic properties which are highly dependent on their size (e.g. Duan et al., 2009; Miller and Shenoy, 2000; Shenoy, 2005; Altenbach et al., 2010; Eremeyev and Morozov, 2010; Goldstein et al., 2010; Shodja et al., 2012).

The size dependency of the mechanical properties at the nanoscale can be understood by incorporating the effect of surface stress. The basic concept of surface/interface stress in solids was first proposed by Gibbs (1906). Later, Gurtin and Murdoch (1975, 1978); Gurtin et al. (1998); Murdoch (1976) elaborated the mathematical framework incorporating surface stress into continuum mechanics. Miller and Shenoy (2000) compared the results obtained by the continuum model with those obtained by means of the embedded atom method for nanobeams and nanowires and found that the results were almost indistinguishable. Basically, the continuum surface stress model assumes that a nanostructure is made of the bulk and some surfaces (Shenoy, 2005) with the surface modules of the nanostructure being different from those of the bulk.

In order to study the effect of surface and interface stresses, numerous boundary value problems have been solved for elastic solids with nano-inhomogeneities, based on Gurtin and Murdoch's theory and generalized Young–Laplace equation (e.g. Tian and Rajapakse, 2007a, 2007b; Mogilevskaya et al., 2008; Kushch et al., 2013; Shodja et al., 2012; Gutkin et al., 2013; Grekov and Yazovskaya, 2013; Bochkarev and Grekov, 2014, etc.). The influence of the surface elasticity on the elastic field even at a planar surface has been reported in Vikulina and Grekov (2012) for the case when the external forces applied to this surface have changed within a nanometer region.

We are cognizant of only a few papers where the surface stress is studied considering nanosized surface asperities (Fu and Wang, 2010; Gill, 2007; Mohammadi et al., 2013; Wang et al., 2010; Weissmuller and Duan, 2008). Gill (2007) has investigated the distribution of the stress at a nanoscale surface flaw in the simplest case, when the surface and substrate have the same elastic properties and the surface stress does not depend on the surface strain and is defined by a determinate function. Owing to such unusual simplifications, he managed to derive an analytical expression for the stress at the surface of an isolated groove of varying sharpness. Following Gurtin and Murdoch's surface elasticity, the elastic field around a single nanosized groove and bugle has been investigated by Fu and Wang (2010) through the finite element method. They found that when the size of the defects shrinks to a nanometer, the stress fields around such defects will be affected significantly by the surface effects. The studies of the other papers listed above have been basically focused on the derivation and analysis of the effective surface stress (Wang et al., 2010; Weissmuller and Duan, 2008) and the effective properties of a nominal flat surface for both randomly and periodically rough surfaces (Mohammadi et al., 2013), but the impact of the surface stress and surface tension on the stress distribution and stress concentration at a roughened surface has not been addressed in those papers.

In the present paper, the approach developed by Grekov (2004, 2011); Grekov and Kostyrko (2013, 2015); Grekov and Makarov (2004); Vikulina et al. (2010) for the analysis of the elastic fields induced by slightly curved surface/interface at the macrolevel is used to study the effect of nanosized surface asperities arising on an initially planar surface. We consider the 2-D problem on the elastic half-space with a slightly curved surface under remote tension and a generalized Young–Laplace boundary condition with unknown surface stress. We solve this problem more completely and correctly than was done in Vikulina (2014). First, we use the boundary perturbation technique and derive the integral dependence of the complex potentials on the surface stress to any-order of approximation. Then, based on the reductive constitutive equations of Gurtin and Murdoch's surface elasticity model, used in a number of publications (e.g. Tian and Rajapakse, 2007a, 2007b; Duan et al., 2009; Altenbach et al., 2010; Shodja et al., 2012; Gutkin et al., 2013, etc.), we satisfy the inseparability condition of the surface and substrate that leads, for an arbitrary surface relief, to the hypersingular integral equation in an approximation of any order of the perturbation method. Similar integral equations have been analytically solved for the half-plane under periodic loading (Vikulina and Grekov, 2012) and a circular nanohole (Grekov and Yazovskaya, 2014) with the appropriate methods. In the first-order approximation, we derive the solution of the integral equation in an explicit form when the surface relief is described by a periodic function, and present formulas for the complex potentials and stress tensor components in the form of complex series. At the end of the paper, we give the most essential numerical results and their analysis for some shapes of the surface.

2. Problem formulation

We consider a semi-infinite elastic solid with a roughened surface slightly deviating from a planar one. The surface has elastic properties differing from the same properties of the volume and, according to the theory of surface elasticity (Gurtin and Murdoch, 1975, 1978), is represented as very thin film which adheres to the bulk material without slipping. The plane strain conditions are assumed to be satisfied and the solid is subjected to a remote tensile loading T and extra surface stress σ_s (Fig. 1).

So, we come to the 2-D boundary value problem for the elastic half-plane $\Omega = \{z : x_2 < \varepsilon f(x_1),\ x_1 \in (-\infty, +\infty)\}$ of the complex variable $z = x_1 + ix_2$ (i is the imagine unit) with the curved boundary $\Gamma = \{z : z \equiv \zeta = x_1 + i\varepsilon f(x_1)\}$.

The function $f(x_1)$ describes the profile of the surface and can be either a continuous periodic function as in Fig. 1, i.e. $f(x_1) = f(x_1 + a)$, or $f(x_1) = 0$ if $|x_1| \geq a$ as in Grekov and Makarov (2004) and Grekov (2011). In the both cases, $\max|f(x_1)| = a,\ \varepsilon|f'(x_1)| < 1,\ 0 < \varepsilon \ll 1$.

As follows from the definition of Γ and f, the maximum deviation of the surface from the plane $x_2 = 0$ is εa.

To obtain the boundary condition at a Γ free from external forces, one can consider the equilibrium of a surface section of infinitesimal length ds on the plane z, as shown in Fig. 2, and unit length in the transverse direction. Besides the surface stresses σ_s and $\sigma_s + d\sigma_s$, the section is subjected to the action of the volume with the net force $\sigma_n ds$ (per unit depth) where σ_n is the traction. Let R, θ be the polar coordinates of the point M and R be the radius of curvature of the arc MN at this point. Then, equating the sum of the x_1 and x_2 projections of all forces to zero and proceed-

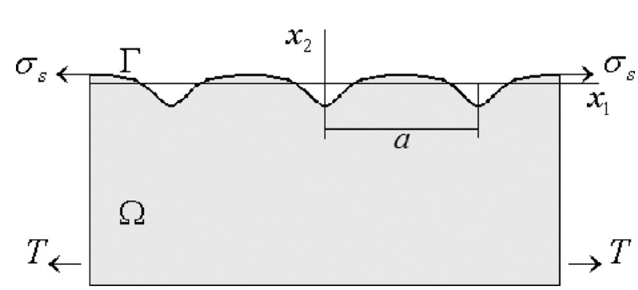

Fig. 1. The model of semi-infinite elastic solid with a nanosized surface asperity.