Tribology International 114 (2017) 161–171

Contents lists available at ScienceDirect

Tribology International

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

On the accurate computation of the true contact-area in mechanical contact of random rough surfaces

Vladislav A. Yastrebov[a,*], Guillaume Anciaux[b], Jean-François Molinari[b]

[a] MINES ParisTech, PSL Research University, Centre des Matériaux, CNRS UMR 7633, BP 87, F 91003 Evry, France
[b] Computational Solid Mechanics Laboratory (LSMS, IIC-ENAC, IMX-STI), Ecole Polytechnique Fédérale de Lausanne (EPFL), Bât. GC, Station 18, CH 1015 Lausanne, Switzerland

ARTICLE INFO

Keywords:
Surface roughness
Contact area
Contact area correction
Simulations
Boundary element method

ABSTRACT

We introduce a corrective function to compensate errors in contact area computations coming from mesh discretization. The correction is based on geometrical arguments, and apart from the contact area itself requires only one additional quantity to be computed: the length of contact/non-contact interfaces. The new technique enables to evaluate accurately the true contact area using a very coarse mesh, for which the shortest wavelength in the surface spectrum reaches the grid size. The validity of the approach is demonstrated for surfaces with different fractal dimensions and different spectral content using a properly designed mesh convergence test. In addition, we use a topology preserving smoothing technique to adjust the morphology of contact clusters obtained with a coarse grid.

1. Introduction

The roughness of natural and industrial surfaces determines properties of the mechanical contact between solids: interface stiffness, true contact area and the morphology of the free interface volume. Thus the roughness governs many interface phenomena such as contact electrical resistance [67,76], thermal contact resistance [41,4], friction [18,6,61], adhesion [23,45], wear [8,2], as well as fluid transport at contact interfaces [42,51,62,15,16,47]. For most of these phenomena it is critical to accurately estimate the true contact area for given thermo-electro-mechanical loads and given roughness of contacting surfaces. It is now well known that a simple load bearing area model, relying on a geometrical overlap of two rough surfaces considerably overestimates the true contact area [46,60], and for equal contact areas, the former results in a much higher transmissivity in transport problems [15]. Existing analytical models, asperity-based [27,9,66,38,26,1], as well as Persson's model [50,52] with its adjusted version [49], rely on a few approximations and thus cannot provide very accurate results in terms of true contact area over a wide interval of loading conditions (for a detailed discussion and comparison see [37,12,44,73,75]).

For these reasons, a numerical analysis, free of restrictive assumptions, is now widely used for the study of rough contact. The following numerical methods are used: the finite element method [46,77], a wide class of continuum boundary element methods [65,54,55,36], discrete methods based on molecular dynamics [10,11,71] or basic molecular dynamics [3,64,45]. Continuum models are particularly attractive since they permit to cover a large spectrum of length scales. However, they are subject to discretization and convergence errors. The former is related to the finite size of the used grid/mesh, whereas the latter is related to the strong non-linearity and discontinuous nature [35,21] of contact problems requiring iterative procedures (Newton-Raphson method, iterative solvers) to achieve convergence, or in the case of explicit techniques for both finite element [29] and the Green's function molecular dynamics [10,11] obtaining the results requires damping of elastic vibrations. Various continuous numerical methods in contact mechanics exist [70], among them penalty and barrier methods, Lagrange multipliers, augmented Lagrangian and other techniques, which convert the constrained optimization problem to an unconstrained one (or at least partially unconstrained). Some of these methods allow accurate satisfaction of contact constraints for a given discretization whereas others (like penalty or barrier type method) only approach the exact solution with an accuracy that depends on the choice of parameters. In addition, different contact discretization techniques, which integrate contact tractions in the weak form in the finite-element method, provide varying accuracy and convergence rates. These depend on the interpolation order of elements, mesh densities on contacting surfaces and mesh curvature. For details, see [70,58,22,69,56,72,19] and references therein.

Assuming that the convergence is ensured and that the numerical

* Corresponding author.
E-mail addresses: vladislav.yastrebov@mines-paristech.fr (V.A. Yastrebov), guillaume.anciaux@epfl.ch (G. Anciaux), jean-francois.molinari@epfl.ch (J.-F. Molinari).

http://dx.doi.org/10.1016/j.triboint.2017.04.023
Received 9 December 2016; Received in revised form 14 April 2017; Accepted 15 April 2017
Available online 18 April 2017
0301-679X/

method is accurate enough, the discretization remains the sole limiting point in achieving accurate results in contact problems. From experience, it is known that for non-conformal but simple geometries (1D or 2D wave, circle or sphere against a flat surface), a rather dense mesh is required at the contact interface to track the contact area evolution, see e.g. [39,40,31,20,77,63]. We also refer to a study of a bi-wavy surface in contact with a rigid flat [74], in which a very dense grid (4096 points per side per wavelength) was used, which allowed the authors to reveal peculiar mean contact pressure behaviour near the percolation point, which was missed in previous studies. Extrapolating to the case of "rough" surfaces, we need to ensure accurate discretization of all harmonics present in the surface spectrum, i.e. the shortest wavelength λ_s should be sufficiently discretized to ensure accurate estimation of the contact area. This statement implies that the surface "roughness" should be smooth enough (or should be smoothly interpolated from experimental data [30,77]) and the ratio $\lambda_s/\Delta x$, where Δx is the grid step, should be kept rather big [73,57]. Importantly, as was demonstrated in [75], the discretization error is affected not only by the shortest wavelength λ_s but also by the longest wavelength λ_l in the spectrum,[1] since it determines the number of individual macro-contact clusters (see [48,75]). Thus, since the error in the true contact area is proportional to the length of the boundary between contact and non-contact zones, a shorter longer-wavelength, results in more contact clusters and leads to a higher discretization error. Hence, for any rough surface with a sufficiently large discrete spectrum, the discretization requirement may rapidly become a bottle neck in terms of computational resources. Two alternative solutions can be used: sacrifice the accuracy by using a coarse mesh and/or use more efficient numerical methods [54,5] and adapted hardware combining CPU and GPU and/or parallel algorithms. A notable example, of combining a Green's function molecular dynamics with computations on GPU enables researchers to make rough contact simulations on a grid with more than 17 billion(!) grid points [57].

The true contact area in numerical simulations of contact can be computed as the total area of surface-faces being in contact plus the areas associated with nodes on the contact-non contact border. In spectral methods [65,36] using FFT techniques and in discrete techniques [10,11] requiring regular discretizations (equally spaced grid points), the true contact area fraction can be simply computed as a ratio between all points in contact (points with zero gap and non-zero pressure) to the total number of points. However, this estimation of the contact area, in general, overestimates the true solution, which could be obtained in the continuum limit. The coarser the discretization, the higher the error: the convergence rate with element size is linear [75].

Here, we suggest an alternative approach that allows an estimation of the true contact area with high accuracy on a reasonably coarse mesh, i.e. enabling full representation of the surface spectrum. The approach is based on a corrective function which uses the length of the contact/non-contact boundary (or simply the perimeter of contact clusters). The method was already introduced in [75], but the previous study lacked a mesh convergence analysis and the corrective factor was not evaluated. Here, we correct these shortcomings and demonstrate the accuracy of the suggested technique on several examples.

The paper is organized as follows: in Section 2, all numerical methods and models are presented: a method used to generate model roughness in Section 2.1, a spectral method used to solve contact mechanical problems in Section 2.2. The area-correction method is described in detail in Sections 2.3 and 2.4. In Section 3, we present mesh convergence tests and demonstrate the performance of the approach. A morphology smoothing of contact clusters is briefly outlined in Section 3.3. A short conclusion is drawn in Section 4.

2. Methods

2.1. Rough surface generation

We use an FFT filtering technique [28] to synthesize an isotropic 2D random rough surface with prescribed Hurst exponent H (or, equivalently, fractal dimension $D = 3 - H$) and cut-offs in the surface spectrum as was done in [73,75]. Note that we use a periodic surface resulting in a discrete spectrum. Surfaces with and without plateau in the power spectral density (PSD) are considered (see [32] for a detailed discussion of PSD measurements and interpretation). The power spectral density is defined as the Fourier transform of the auto-correlation function and using the convolution theorem can be written through the Fourier transform of the surface $z(x, y)$:

$$\Phi_s(k_x, k_y) = \hat{z}(k_x, k_y)\hat{z}^*(k_x, k_y), \tag{1}$$

where the star denotes the conjugate value and the hat denotes the Fourier transformed quantity:

$$\hat{z}(k_x, k_y) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp[-i(k_x x + k_y y)]z(x, y)dxdy. \tag{2}$$

One can compare surfaces with plateau depicted in Fig. 1(c), (e) with those without it, see Fig. 1(d), (f). The surface PSD is characterized by the following parameters: a scaling factor Φ_0, Hurst exponent H, absence or presence of a plateau and also two wavenumbers k_l and k_s: k_l the lowest wavenumber determining the start of a power-law decaying PSD and k_s the highest wavenumber determining the shortest wavelength present in the spectrum. The mean profile PSD[2] for a surface with and without plateau can be formalized in the following forms, respectively:

$$\Phi_p(k) = \begin{cases} \Phi_0, & \text{if } k \le k_l (\text{plateau}) \\ \Phi_0(k/k_l)^{-2(H+1)}, & \text{if } k_l < k \le k_s \\ 0, & \text{else} \end{cases},$$

$$\Phi_p(k) = \begin{cases} \Phi_0(k/k_l)^{-2(H+1)}, & \text{if } k_l < k \le k_s \\ 0, & \text{else} \end{cases}, \tag{3}$$

where $k = \sqrt{k_x^2 + k_y^2}$, with k_x,k_y are wavenumbers in x and y directions ($k_{x,y} = 2\pi/\lambda_{x,y}$), respectively, and

$$\Phi_p(k) = \frac{1}{2\pi}\int_0^{2\pi}\Phi_s(k_x, k_y)d\phi = \frac{1}{2\pi}\int_0^{2\pi}\Phi_s(k\cos(\phi), k\sin(\phi))d\phi$$

is the mean profile PSD for a given absolute value of the wavevector k in all directions determined by ϕ. The surface is considered to be isotropic, so that statistical characteristics of every profile should be independent of the direction ϕ. Since we deal with a discrete spectrum the integral in the previous expression should be rewritten as:

$$\Phi_p(k) = \frac{1}{n(k)}\sum_{\forall k_x, k_y : k_x^2 + k_y^2 = k^2}\Phi_s(k_x, k_y),$$

where $n(k)$ is the number of elements satisfying $k_x^2 + k_y^2 = k^2$ for all $k_x, k_y \in \mathbb{Z}$. Because of this discreteness, the accuracy of definition (3) cannot be satisfied for a single surface. Thus, multiple realizations of rough surfaces for a given set of parameters k_l, k_s, H is needed to capture the statistical nature of the roughness. It is convenient to introduce dimensionless wavenumbers $\tilde{k}$, which will be used throughout the paper:

$$\tilde{k} = kL/2\pi = L/\lambda,$$

where λ is the wavelength and L is the length of a side of simulation box. It means that $\tilde{k}$ is the number of waves per length, and because of the periodicity this quantity takes only integer values. Some examples

[1] For surfaces with a plateau in the surface spectrum, λ_l corresponds to the shortest wavelength present in the plateau as in examples shown in Fig. 1(c-e).

[2] Lower index "p" is used for profile PSD and lower index "s" is used for surface spectrum.