Van der Waals Force Computation of Freely Oriented Rough Surfaces for Micromanipulation Purposes

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Abstract—This paper describes a numerical method to compute van der Waals force between complex and freely oriented objects that have rough surfaces. The force calculation is implemented using the surface formulation of the force. First, the interacting surfaces are approximated with triangular meshes. Then, the surface roughness is taken into consideration by separately adding the asperity heights to each point of the smooth reference surfaces. Three different models are used to describe the rough surfaces: sinusoidal, fractal, and probabilistic. All the three models show considerable reduction in the force values as a function of the roughness peak height or the inclination angle of the surfaces, van der Waals force is considered to be an essential part when calculating the total interaction force for micromanipulation purposes.

I. INTRODUCTION

LL ENGINEERING surfaces are rough at some level. At microscale, even small surface asperities influence the forces that govern the object interaction. Therefore, it is essential to take roughness into consideration in the microsystem design. In this paper, the intended application roughness calculations is area of the contact micromanipulation. The term "micro" refers to object sizes below hundreds of micrometers and contact micromanipulation means that the tool physically touches the objects during manipulation.

Due to the so called scaling effect [1, 2], the three forces that dominate the interaction at microscale are van der Waals force, capillary force, and electrostatic force [3]. These surface forces make micromanipulation differ considerably from manipulation at the conventional macroscale. Each one of the three forces is affected by the surface roughness. Van der Waals force in particular is sensitive to surface roughness since the force values depend strongly on the distance between the interacting objects. In this paper, the emphasis will be entirely on van der Waals force.

In terms of interaction force *models*, the manipulationspecific requirement is the applicability of the models to complex object shapes *and* arbitrary object orientations. This kind of models could be implemented for manipulation design (e.g., design of manipulation strategies, or endeffectors), for simulator development, and sometimes even for manipulation control.

Many types of van der Waals force models for perfectly smooth surfaces have been presented in the literature. Proposed approaches include both analytical (e.g., [3, 4]) and numerical models (e.g., [5, 6]). However, only a few of the published models (e.g., [7, 8]) satisfy the manipulationrelated requirements concerning the freedom of shape and orientation of interacting objects.

An analytical method to include the effects of roughness in the van der Waals force evaluation was presented in [4]. The method takes into consideration the height of the highest roughness peak but not the density of the peaks. Alternative approaches utilize elementary shapes to model the asperities, e.g., spheres and cones [9, 10]. In addition, sinusoidal functions have been considered [11]. Other interesting approaches to surface roughness modeling at micro- and nanoscales can be found in tribology. In tribology, the roughness models are categorized to probabilistic models (e.g., Gaussian) [12] and fractal models [13, 14]. In these approaches, roughness models are typically developed for two nominally flat parallel surfaces.

As shortly discussed above, literature shows some methods to compute van der Waals force for complex object shapes having arbitrary orientations and other methods to include surface roughness in the force values. However, it seems that no method published this far discusses how to combine these two important features for van der Waals force. A model that takes into account both surface roughness and freedom of orientation would be very valuable for micromanipulation purposes.

This paper proposes a numerical method to compute van der Waals force for freely oriented rough surfaces. The rest of the paper is organized as follows. First, Section II presents the parameterization that allows calculations for arbitrary shapes and orientations for smooth surfaces. The different models to present rough surfaces and their inclusion to the force model are presented in Section III. Section IV gives force results and Section V discusses the issues related to modeling. Section VI concludes the paper.

II. FORCE CALCULATION BETWEEN SMOOTH SURFACES

In case of pairwise additivity and nonretarded forces, the van der Waals force between two objects can be calculated using the so called Hamaker's approach [15, 16]. This leads to the volume formulation of the force, i.e., the total force F_{vdW} is

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$$F_{vdW} = \rho_1 \rho_2 \int_{V_1} \int_{V_2} \nabla w dV_1 dV_2 , \qquad (1)$$

where ρ_i and V_i refer to the number density and volume of the interacting object i = 1, 2, and ∇_w stands for the van der Waals force between a pair of atoms or small molecules, one taken from each of the interacting volumes.

In our work, we have adopted the surface formulation [6] for the van der Waals force. When compared to the conventional volume formulation, the surface formulation reduces the 6-dimensional integral in (1) to a four dimensional one. This change significantly reduces the computational complexity that is involved in the force evaluation. Surface formulation gives the total force F_{vdW} between two interacting objects as follows [6]

$$\boldsymbol{F}_{vdW} = \boldsymbol{\rho}_1 \boldsymbol{\rho}_2 \int_{S_1} \int_{S_2} (\boldsymbol{G} \cdot \boldsymbol{n}_1) \cdot \boldsymbol{n}_2 dS_1 dS_2 , \qquad (2)$$

where S_i and n_i represent the boundary surface and outward pointing unit normal of object i = 1, 2, respectively. The function *G* depends on the relative orientation of the objects and on their distance from each other, i.e.,

$$G = \frac{C\mathbf{x}}{3(\mathbf{x} \cdot \mathbf{x})^3},\tag{3}$$

where *C* is a material dependent constant and x is a vector from point x_{2l} on surface S_2 to point x_{1k} on surface S_1 (see Fig. 3a). The integration in (2) goes over all points on each surface.

In our previous work, we applied the surface formulation in a parametric domain, which enables the force evaluation between complex object shapes and arbitrary orientations [7, 17]. Parameterization of the surfaces is implemented by approximating the surfaces with triangular meshes. For a pair of interacting triangles, the force in (2) takes the following form

$$F_{T} = \rho_{1}\rho_{2} \int_{0}^{(1-\nu_{1})} \int_{0}^{1} \int_{0}^{(1-\nu_{2})} \int_{0}^{1} G \cdot (E_{11} \times E_{12})$$

$$\cdot (E_{21} \times E_{22}) du_{1} dv_{1} du_{2} dv_{2},$$
(4)

where E_{ij} means edge j = 1, 2 on triangle i = 1, 2 and the subscript T in F_T refers to the van der Waals force between two triangles, one from each of the interacting surfaces. The total van der Waals force F_{vdW} is then obtained by summing



Fig. 1. A triangle taken from the surface approximation of object 1 a) using Cartesian coordinates and b) the parameterized triangle.

together all the intermediate results from different triangle pairs. After the parameterization, the vector x in (3) becomes

$$\mathbf{x} = \mathbf{x}_{2l} - \mathbf{x}_{1k} = \mathbf{V}_{20} + u_2 \mathbf{E}_{21} + v_2 \mathbf{E}_{22} - \mathbf{V}_{10} - u_1 \mathbf{E}_{11} - v_1 \mathbf{E}_{12}, \quad (5)$$

where V_{0i} refers to a vertex point between edges E_{ij} on triangle *i* and u_i and v_i are variables in the parametric domain for triangle *i* (see Fig. 1).

In practice, the force evaluation using (4) requires numerical computation (applies to (1) and (2) as well). We have used a lattice method to solve the numerical quadrature [18]. In a few special cases, an analytical solution to the van der Waals force in (1) can be found. An example of a closed form solution is the force for a unit area between two infinite (parallel) planes at distance d from each other

$$F_{vdW} = \frac{H}{6\pi d^3},\tag{6}$$

where *H* is the material dependent Hamaker constant that depends on *C* and on the number densities ρ_i in the following way

$$H = \pi^2 C \rho_1 \rho_2 \,. \tag{7}$$

The few existing analytical solutions are useful since they can be utilized for validating the numerical results. When comparing the force values from (4) to analytical solutions, the numerical method gives satisfactory results, especially for flat surfaces (see also Fig. 4, Fig. 5, and Fig. 8). For curved surfaces, the method suffers from inaccuracies that are caused by the inability of triangles to approximate curved surfaces [7, 17]. This problem can be reduced by increasing the number of surface-approximating-triangles.

III. MODELS FOR ROUGH SURFACES

In this paper, we consider two types of rough surfaces: 1) deterministic surfaces that are homogeneous and isotropic and 2) random surfaces. For random surfaces, two different approaches are chosen: 1) a fractal surface presentation where the force calculation directly utilizes the topography information in order to form vector x in (5) and 2) a probabilistic surface presentation where the peak height is regarded as a random variable having Gaussian distribution and the asperity height at each point of the surface is given by a probability density function.

Deterministic surfaces are generated using sinusoidal functions so that the peak height z at each point (x, y) on the surface is given as

$$z(x, y) = \left[\sin^2(x\pi f_1) + \cos^2(y\pi f_2) - 1\right] \cdot a, \tag{8}$$

where frequency f_i gives the number of signal periods on edge *i* and *a* is the amplitude of the peaks. When considering engineering surfaces, this type of a surface topography may seem unrealistic. However, it allows a straightforward way to study the effects of peak height and peak density on van der Waals force.

Fractal surfaces are generated by using the Weierstrass-Mandelbrot (W-M) fractal function [19]. A threedimensional surface can be generated by using a modified two-variable W-M function. It gives the peak height z at each point (x, y) on the surface as follows [20]

$$z(x, y) = L(\frac{G}{L})^{D-2} \left(\frac{\ln \gamma}{M}\right)^{\frac{1}{2}} \sum_{m=1}^{M} \sum_{n=1}^{n_{max}} \gamma^{(D-3)n} \cdot \left\{\cos(\phi_{m,n}) - \cos\left[\frac{2\pi\gamma^{n}(x^{2}+y^{2})}{L}\cos\left(\tan^{-1}(\frac{y}{x}) - \frac{\pi n}{M}\right) + \phi_{m,n}\right]\right\},$$
(9)

where G is the fractal roughness that affects the amplification of the surface peaks and valleys (independent of the frequency), D is the fractal dimension that determines the contribution of the high and low frequency components on the surface (high value of D indicates that high-frequency components dominate over low frequency components), M is the number of superposed ridges that are used to construct the surface, γ is a scaling parameter (a good value is $\gamma = 1.5$), and $\phi_{m,n}$ is a random phase. Furthermore, L is the length of the sample profile, n is the frequency index $(n_{\text{max}} =$ $\log(L/L_s)/\log\gamma$ and n_{\max} is an integer), and L_s is the cut-off length referring to the resolution at which the asperities can be detected. Values for the material dependent parameters can be found in the literature. We have used values for LIGA nickel [21]: D = 2.4815, G = 1.3152 nm, $L_s = 1.47$ nm, M = 10. In our case, the lengths of the small sides of a right triangle are 1 μ m, thus $L = 1 \mu$ m. Fig. 2 gives examples of a fractal surface and a surface that is generated using sinusoidal functions.

For a probabilistic Gaussian model [12], the probability density function $\phi(z)$ of the roughness peak height z is

$$\phi(z) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(z^2/2\sigma^2)},$$
 (10)

where σ is the standard deviation of the asperity heights. The height *z* is perpendicular to the mean line of the surface as shown in Fig. 3 (applies to other roughness models as well).

The implementation of surface roughness models with parameterized surfaces is elucidated in Fig. 3 for a twodimensional case. For smooth surfaces, the vector \mathbf{x} between any two points \mathbf{x}_{2l} , \mathbf{x}_{1k} taken from the surfaces 1, 2 is the difference between the points, i.e., $\mathbf{x} = \mathbf{x}_{2l} - \mathbf{x}_{1k}$. In case of rough surfaces, also the height of the roughness peak at each point has to be taken into consideration. The roughness peak height is obtained from equations (8)–(10), or from any other appropriate model. The direction of the roughness peak



Fig. 2. Examples of rough triangle surfaces: a fractal surface (upper) and a surface that is created by using sinusoidal functions (lower).

is then determined by the unit-length normal n_{1u} of the surface. Thus, the vector x from point k on the rough surface 1 (i.e., triangle 1 in this case) to point l on the smooth surface 2 (triangle 2) becomes

$$x = x_{2l} - x_{1k} - zn_{1u}.$$
(11)

For the sinusoidal and the fractal roughness models, the force calculation between rough surfaces requires the addition of asperity heights in the distance calculations (i.e., in the calculation of x, as shown in (11)). After this addition, equation (4) can be used for the force evaluations. In case of the probabilistic model, the probability density function has to be included in the calculations. According to [12], the van der Waals force is calculated as follows

$$F_{vdW} = A \int_{-\infty}^{n-\varepsilon} f_{vdW}(h-z)\phi(z)dz, \qquad (12)$$

where ε is the equilibrium distance for flat surfaces at contact (e.g., $\varepsilon = 0.2$ nm), h is the separation distance between a smooth surface and the mean line of a rough surface (see Fig. 3b), f_{vdW} is the closed form solution for van der Waals force between two infinite parallel planes (force for a unit area), and A is the contact area of the interacting surfaces. In (12) the van der Waals force is solved analytically for the smooth case and thus, the force calculation requires numerical computations only in one dimension. In our case, the freedom in object orientation requires that also the force between smooth surfaces is calculated numerically. Therefore in our calculations, the $f_{\rm vdW}$ in (12) is replaced with equation (4) and since the area is implicitly included in (4), the factor A in (12) is removed. Although not implemented in here, the model in (12) can be augmented to take into consideration also the spatial distribution of the roughness peaks [12].

IV. FORCE RESULTS

In the following, results that are obtained with different roughness models are presented. In each case, the interacting objects are two right triangles with two identical small sides that have length of 1 μ m. The Hamaker constant used in the calculations is 1×10^{-19} J. Unless otherwise stated, the numerical integration is carried out by using a lattice method [18].



Fig. 3. A vector x in 2D that connects two points taken from the interacting surfaces. a) Two smooth surfaces and b) a smooth surface and a rough surface. The dotted line in 3b) represents the mean surface.

A. Sinusoidal surfaces

Fig. 4 depicts van der Waals interaction force as a function of the separation distance between a smooth triangle and a parallel rough triangle. The rough surface topography is generated with sinusoidal functions according to (8). The separation distance h between the smooth surface and the mean line of the rough surface is defined as h = d + da, where a is the amplitude of the roughness peak (i.e., the maximum height of the peak above the mean line) as shown in Fig. 4. The results are given for three different peak heights a (1 nm, 10 nm, and 100 nm) and for two different peak densities (4 and 40 periods on each small side). For comparison, also the results for smooth surfaces are shown-both analytical and numerical. The analytical results are obtained by applying (6) for same sized area as the interacting area between the triangles. This result is not directly comparable since it gives the force for certain area taken from infinite planes and in case of triangles the interacting areas are obviously finite. The difference is emphasized at larger separation distances.

It is shown that surface roughness has a rather dramatic effect on the force values. At the separation distance of 1 nm and with roughness peak heights of 100 nm (peak density is 40), the force value is almost 16000 times bigger for smooth surfaces than for a smooth surface interacting with a rough one. With a lower roughness peak height of 10 nm, the force is still over 400 times bigger for smooth surfaces than for a smooth and a rough surface. Also the roughness peak density has an effect on the force values. With fewer roughness peaks, the area that is at minimum distance from the smooth surface is smaller than with higher peak density, thus lowering the van der Waals force value. The results also indicate that the effect of roughness loses its effect at a point where the separation distance becomes larger than ten times the value of the asperity height (i.e., force values for rough surfaces approach the force values for smooth surfaces).

Most of the results presented in this paper are obtained for a smooth surface interacting with a rough one. This is based



Fig. 4. Van der Waals force as a function of the separation distance.
 A smooth triangle interacting with a rough one. Effects of roughness peak density and peak height on the force (sinusoidal roughness peaks). For comparison, the force values are also presented for smooth surfaces (analytical and numerical results).



Fig. 5. Van der Waals force as a function of the inclination angle α . A smooth triangle interacting with a rough one. Effect of roughness peak height and separation distance on the force (sinusoidal roughness peaks). For comparison, the force values are also presented for two smooth surfaces (numerical results).

on the idea that two rough surfaces can be presented as a smooth surface and an equivalent rough surface. The variance and the mean of the equivalent surface are equal to the sums of the means and variances of the actual rough surfaces [12]. For comparison, Fig. 4 gives an example of a situation where both interacting surfaces are rough.

In Fig. 5, the van der Waals force is presented as a function of the inclination angle α when one of the surfaces is tilted. Tilting takes place relative to one of the small edges. The results are presented for two different separation distances d (1 nm, 100 nm) and for two different roughness peak heights a (1 nm, 10 nm). For comparison, also the force results between two smooth triangles are presented.

B. Fractal surfaces

Examples of force results as a function of the separation distance for fractal surfaces are presented in Fig. 6. In the calculations, values for LIGA nickel are used as the material dependent parameters (see Section III).

With random surfaces, the determination of the separation distance in the same way as for the deterministic surfaces in Section IV.A produces lower force values (for identical values of d). This is due to the fact that on a random surface, all the peak heights do not have the same maximum value and the asperities are not evenly distributed on the surface. In Fig. 6, the results are given using three different approaches to calculate the separation distance. In each case, the mean value of the roughness peaks is zero. In other words, at zero lies the smooth reference surface and the asperity heights are added to this value. The three different approaches to calculate the distance are: 1) distance between the smooth surface 2 and the mean of the rough surface 1 is $h = d + \sigma$, where σ is the standard deviation of the roughness peaks, 2) distance between the smooth surface 2 and the mean of the rough surface 1 is $h = d + 2\sigma$, and 3) the separation distance between the smooth surface 2 and the mean of the rough surface 1 is $h = d + z_{max}$, where z_{max} refers to the maximum roughness peak height. In Fig. 6, the values



Fig. 6. Van der Waals force as a function of the separation distance for parallel surfaces. A smooth triangle interacting with a rough one (fractal surface). Separation distance between the surfaces is determined in three different ways. Symbol σ refers to the standard deviation of the roughness peak heights.

for σ and z_{max} are 2.39x10⁻⁸ m and 4.21x10⁻⁷ m, respectively.

Except for the third case presented above, the method to calculate the separation distance means that parts of the interacting surfaces are in contact as shown in Fig. 6. The calculation of the vector x in (11) does not prevent the roughness peaks from penetrating the interacting surfaces. Thus, the contact situation has to be considered separately. In our approach, the height of the roughness peaks that exceed the separation distance between the interacting surfaces is fixed to a value $h - \varepsilon$, where h is the separation distance between the surfaces at that point (between the smooth surface and the mean line of the rough surface, see Fig. 3b and Fig. 7) and ε is the interatomic equilibrium distance (here, $\varepsilon = 0.2$ nm). In other words, in contact, the highest peaks are cut by the smooth surface. At those points, the force has its maximum value (force at the equilibrium distance).

For parallel surfaces, the determination of the separation distance h between them is trivial. For arbitrary orientations, when a rough surface is interacting with a smooth one, the calculation of h is done as follows

$$h = \left\| \frac{V_{02} \cdot (\boldsymbol{E}_{21} \times \boldsymbol{E}_{22}) - \boldsymbol{P} \cdot (\boldsymbol{E}_{21} \times \boldsymbol{E}_{22})}{(\boldsymbol{E}_{11} \times \boldsymbol{E}_{12}) \cdot (\boldsymbol{E}_{21} \times \boldsymbol{E}_{22})} \right\|,$$
(13)

where V_{02} is a vertex point on triangle 2, P is a point on triangle 1, $(E_{i1} \times E_{i2})$ is the surface normal of triangle *i*, and $\|\|\|$ is a norm that gives the length of the vector. The distance calculation is presented in Fig. 7. The method is only suited for a rough surface interacting with a smooth one. In case of two rough surfaces, the distance evaluation depends on more than two points. Thus, also the neighboring points have to be taken into consideration.

C. D. Probabilistic surfaces

In Fig. 8, results obtained with the probabilistic model and Monte Carlo integration [22] are presented. Force results are



Fig. 7. At point *P* on triangle 1, the maximum height *h* of the roughness peak is limited by the surface *S* spanned by the edges of triangle 2. In case of non-convex surfaces, also the neighboring triangles affect *h*.



Fig. 8. Surface roughness as a stochastic process. Probabilistic model (Gaussian), where the peak height is a random variable. Hariri-model [12] is intended for infinite flat surfaces at close distances (numerical integration in only one dimension, see (12)).

shown as a function of the separation distance for parallel surfaces and for a situation where the smooth surface is tilted. Separation distance is calculated between the smooth surface and the mean line of the rough surface. The results are compared to those obtained by using (12) for two parallel infinite planes (i.e., numerical integration is implemented only in one dimension since the van der Waals force for parallel infinite planes can be evaluated in closed form). In all of the simulations, the equilibrium distance ε is 0.2 nm and the standard deviation σ is 10.315 nm, which is the value for gold surface as given in [12]. The penetration of the roughness peaks to the interacting surface is detected in a similar way as for the fractal surfaces, e.g., using (13).

V. DISCUSSION

Many engineering surfaces can be considered as fractal (see, e.g., [22]) which justifies the use of fractal surface model in van der Waals force evaluation. For the probabilistic model, other peak height distributions besides Gaussian can be used. This augments the applicability of the model for many types of rough surfaces. The roughness model that utilizes sinusoidal functions has low resemblance with real engineering surfaces. However, it gives straightforward means to examine the effect of roughness peak height and spatial peak density on the force values.

Common problem with all the three roughness models is

the high computational complexity that is involved in the force evaluation. This is caused by the highly nonlinear integrand combined with the complex surface topography. The numerical integration for sinusoidal and fractal surfaces was implemented with a lattice method [18], that used approximately 320000 function evaluations. The fractal model is computationally more demanding than the sinusoidal model since the (rough) surface formation is more complicated and the penetration of roughness peaks to the interacting surface has to be separately detected (applies to the probabilistic model as well). In case of the probabilistic model, computational complexity is further increased by the additional (fifth) integration dimension that is required when compared to the other two methods. The lattice method with 320000 function evaluations did not produce reliable results. Thus, the results in Section IV.C were obtained with Monte Carlo integration [23] using up to 10^9 function evaluations. The computational complexity makes the probabilistic model inefficient for larger objects (when the dimensions are measured in hundreds, or even tens, of micrometers).

An advantage of the probabilistic model is that there is no need to separately generate the rough topography during force calculations. Therefore, the shape of the interacting surfaces or the selection of the function evaluation points cannot affect the force results in the same way as with the sinusoidal or the fractal model.

The presented force calculation method—independent of the used surface roughness model—is especially suited for surfaces that can be divided into flat sub-surfaces. For curved surfaces, the triangular surface approximation leads to errors as discussed in Section II. This problem can be overcome with different surface approximations, e.g., with splines [8].

Better applicability of the proposed method for micromanipulation purposes requires further research efforts at least in the following four areas: 1) reduction of the computational complexity, 2) better force models, e.g., in terms of the retardation effect (here, the Hamaker's approach was obtained in order to have analytical reference results the method in itself is not restricted to Hamaker's approach), 3) validation of the results with measurement data, and 4) combination of the force values with those representing capillary force and electrostatic force in order to get the total force values.

VI. CONCLUSIONS

This paper presented approaches to calculate van der Waals force between two objects that have complex shapes, rough surfaces, and arbitrary orientations relative to each other. The surfaces of the interacting objects were approximated with triangular meshes and three different surface roughness models: sinusoidal, fractal, and probabilistic. The force results showed that already small asperities and small inclination angles can considerably decrease the effect of van der Waals force in object interaction. The results also indicated that beyond a certain separation distance, the roughness has no effect on the force values. Furthermore, the asperity peak height seems to have a greater impact on force values than the peak density.

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