EFFECTS OF SUBSTRATE ROUGHNESS ON VAN DER WAALS AND ELECTROSTATIC FORCE CONTRIBUTIONS TO PARTICLE ADHESION

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ABSTRACT: We characterize the effect of substrate roughness on van der Waals and electrostatic particle adhesion forces using theoretical methods. We find that substrate roughness can enhance or diminish electrostatic adhesion by at maximum a factor of ~2 for the surfaces studied, but can attenuate van der Waals forces by several orders of magnitude. Thus, substrate roughness can change the dominant contribution to adhesion from van der Waals forces to electrostatic forces.

KEYWORDS: particle adhesion, roughness, electrostatics, van der Waals

1. INTRODUCTION

In dry systems, particle adhesion to surfaces is governed by van der Waals and electrostatic forces. Van der Waals forces are expected to dominate particle adhesion to flat surfaces for most relevant systems (Mittal & Jaiswal, 2015). However, all surfaces have some degree of roughness which significantly alters the degree of adhesion. Since van der Waals and electrostatic forces have different functional dependencies, surface roughness will have different effects on each, and may alter which force is dominant for adhesion. Here we investigate the effect of surface roughness on electrostatic adhesion and compare this to van der Waals forces in rough systems.

The effect of surface roughness on van der Waals forces has been studied extensively. In most systems, surface roughness reduces van der Waals forces by diminishing the contact area between surfaces (Rajupet, Sow, & Lacks, 2020). However, in cases where particles adhere within valleys, the van der Waals force has been shown to increase due to enhanced contact area (Kumar, Staedler, & Jiang, 2013).

Comparatively few studies have investigated the effect of surface roughness on electrostatic adhesion. Studies found that surface roughness enhances the electrostatic adhesion force by increasing the area of the rough surface, and thereby the charge and capacitance (Feshanjerdi, 2020; Feshanjerdi & Malekan, 2019). However, charge concentrates on peaks of rough surfaces (Fricker, 1989), enhancing the electric field at peaks and diminishing the electric field in valleys of the rough surface, an effect prior studies did not account for.

Here we investigate the effect of surface roughness on electrostatic particle adhesion while accounting for polarization in a dielectric material and charge redistribution on a conducting surface. We study the interaction between a charged dielectric particle and a grounded rough substrate. To simplify the system, we assume that the particle is spherical, has a uniform charge density, and is positioned directly above an asperity. This system is of particular interest for loss of vacuum scenarios in Tokamak fusion reactors, where adhesion forces between tungsten particles coated with thin oxide layers and rough tungsten metal surfaces govern the degree of hazardous dust dissemination into the environment.

2. METHODOLOGY

The calculation of the electrostatic force between the particle and surface proceeded by the following steps: (a) solve Poisson's equation for the electrostatic potential; (b) obtain the electric field from the electrostatic potential; (c) use the electric field results to determine the Maxwell stress tensor; and (d) integrate the Maxwell stress tensor over the surface of the particle to obtain the electrostatic force. Poisson's equation is solved using a finite element method with a variable size mesh, with the system constrained within a cylindrical calculation cell. The bottom surface of the calculation cell corresponds to the physical rough substrate with which the particle interacts, and has the boundary condition ϕ = 0, where ϕ is the potential. The sides and top of the calculation cell have the boundary condition $\nabla\phi = 0$. The residual space in the calculation cell is vacuum with permittivity ε_0. The size of the calculation cell was varied such that the boundaries have a negligible effect on the calculation results. The COMSOL Multiphysics simulation package is used to carry out the calculations.

The rough surface is approximated as a sinusoidally varying landscape,

$$z(x,y) = A\left[\frac{1}{2}\sin(2\pi \mathrm{x}/\lambda) + \frac{1}{2}\sin(2\pi \mathrm{y}/\lambda)\right] \quad (1)$$

where *z* is the height of the surface as a function of the coordinates x and y, and *A* and λ are the amplitude and wavelength of the function describing the surface roughness. We model the dielectric particle as a sphere with radius, *R*, permittivity, ε, and uniform surface charge density σ, separated from the rough surface by the contact distance, d_c, which we assume is 0.5 nm. To make the exploration of parameter space feasible, we consider only particle positions directly above an asperity.

We compare the effect of roughness on electrostatic forces to that on van der Waals forces. To determine the van der Waals force on a particle due to a rough substrate, F_V, we use an analytic model that we developed in our previous work. Unlike previous models, this model takes into account particle interactions with multiple asperities on the rough surface (Rajupet, Sow, & Lacks, 2020):

$$F_V = \frac{HR}{6d_c^2}\left(\frac{1}{1+R/R_a} + \frac{16\pi d_c^2 (R+R_a+d_c)^2}{\lambda^2(1+R/R_a)(\lambda^2+8d_c(R+R_a+d_c))}\right) \quad (2)$$

Here, *H* is the Hamaker constant which depends on the composition of the interacting objects and medium, and R_a is the radius of curvature of asperities on the surface. For a sinusoidal, surface $R_a = \lambda^2/2\pi^2 A$. Using this model, we found very good agreement with exact theoretical van der Waals forces. Similar to our electrostatic force calculations, this model is derived for a particle positioned directly above an asperity.

3. RESULTS

A charged dielectric particle in the vicinity of a grounded substrate induces an image charge of opposite polarity in the substrate. The electric field due to the image charge polarizes the particle. The image of this polarization induces higher order polarizations and this process continues *ad infinitum*. The electrostatic force between a spherical dielectric particle and a flat grounded substrate has previously been determined (Matsuyama & Yamamoto, 1998). The electrostatic force we calculate for the flat substrate system agrees very well with past results, thus verifying our computational methodology.

We now apply our methodology to determine the electrostatic and van der Waals forces between a particle and a rough substrate. Figure 1a shows the rough substrate force normalized by the smooth substrate force for both the electrostatic and van der Waals interactions. Thus, Fig. 1a represents the enhancement or attenuation of the adhesion force due to substrate roughness. Note that the normalized adhesion forces do not depend on the surface charge density, σ, or the Hamaker constant, *H*.

We first address the qualitative behavior of the normalized adhesion force for increasing particle radius. When *R* is very small relative to R_a, both the van der Waals and electrostatic normalized forces approach 1. In this limit, the surface asperities "appear" flat to the particle causing the rough substrate force to approach the smooth substrate force. As *R* increases but is still $\lesssim R_a$, the electrostatic force is enhanced. In this regime, the particle only interacts with the asperity directly below it and is not big enough to interact significantly with valleys of the surface. The electric field in our system is enhanced near peaks of the rough surface and diminished near valleys, causing the electrostatic adhesion force to be enhanced when the particle interacts more significantly with peaks.

As the radius continues to increase, the particle begins to interact significantly with valleys of the rough surface where the electric field is attenuated; in this regime, the electrostatic force is diminished. Again, as the particle size increases, the particle interacts with more peaks, thereby increasing the normalized electrostatic adhesion force. Due to computational limitations, we could not calculate the electrostatic adhesion force for larger particle sizes. We expect that as the radius continues to increase and the particle sequentially interacts with more peaks and valleys, the normalized electrostatic adhesion force will exhibit a dampened oscillation. In the limit that *R* goes to infinity, the bottom half of the particle will resemble a flat surface. We can simulate this case using a charged dielectric flat surface interacting with a grounded rough substrate. In this limit, whether the electrostatic force is enhanced or diminished depends on the substrate morphology and the permittivity of the particle.

The van der Waals adhesion force continues to diminish as the particle size is increased. Since the van der Waals force is a shorter range force than the electrostatic force, the particle must be much larger to begin interacting significantly with other peaks of the rough substrate. At very large particle sizes, the normalized van der Waals adhesion force stabilizes as it interacts with several peaks on the rough substrate.

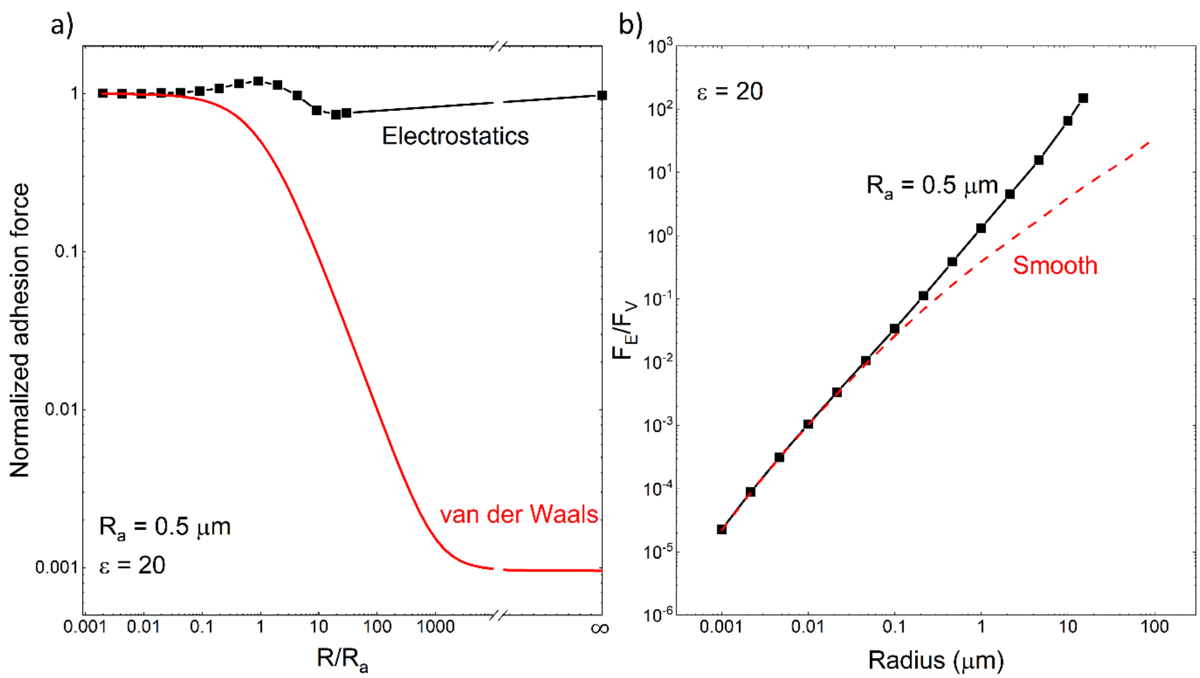

Figure 1: a) The force on a particle due to a rough substrate normalized by the flat substrate force, as a function of *R* for the van der Waals force (red line) and the electrostatic force (black points), b) The ratio of the electrostatic force, F_E, to the van der Waals force, F_V, for a rough surface (black points) and a smooth surface (red dashed line) for a particle with σ of 300 µC/m^2 and an *H* of 4×10^{-19} J . For both a) and b) the particle permittivity is 20 and the radius of asperity of the rough surface, R_a, is 0.5 µm, corresponding to a substrate with λ = 1 µm and *A* = 0.1 µm.

4. DISCUSSION

To contextualize our results, we compare the magnitudes of the rough substrate electrostatic and van der Waals forces. Figure 1b shows the ratio of electrostatic to van der Waals forces, F_E/F_V, for a particle interacting with a rough substrate. The particle has a uniform σ of 300 µC/m^2 and permittivity, ε, of 20, a characteristic permittivity for dielectric particles. The Hamaker constant we used for this system is 4×10^{-19} J, typical of tungsten particles and substrates interacting in air.

At small particle sizes, the van der Waals force dominates adhesion. As the particle size increases, electrostatic forces become more prominent, and dominate at large particle sizes. Figure 1b shows that surface roughness can decrease the particle size where electrostatic forces are comparable to van der Waals forces by nearly an order of magnitude. This is because substrate roughness only scales

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(increases or decreases) the electrostatic force by at maximum, a factor of ~2. On the other hand, substrate roughness can diminish the van der Waals force by several orders of magnitude.

We emphasize that our results in Fig. 1b can be generalized for any σ and H since, even for rough surfaces, the electrostatic force scales with σ^2 and the van der Waals force scales with H. Here, we used a σ in the upper limit of reasonable surface charge densities. However, we note that for surfaces in contact, this may be an average or even low surface charge density, since typical charge measurements are made after surface separation and charge has backflowed between the surfaces (Shen, Wang, Sankaran, & Lacks, 2016).

For particle sizes less than R_a, we expect that the adhesion force will depend significantly on particle position on the surface since, in this size regime, particles can adhere anywhere on the surface, i.e. either above peaks or in valleys of the rough surface. Here, we only considered particles positioned directly above a peak of the surface. Preliminary results show that the electrostatic force is diminished for particles positioned in valleys of the rough surface, and previous studies have shown that the van der Waals force is enhanced in this case (Kumar et al., 2013). For larger particle sizes, we expect particle position to be less significant since, in this regime, particles cannot fit in valleys of the surface. Furthermore, in real systems, substrates have multiple scales of roughness simultaneously and particles can have irregular morphologies. Here, our results provide an insightful first order approximation of the effect of roughness on adhesion forces for these more complex real systems.

5. CONCLUSIONS

We use theoretical analysis to address the effect of substrate roughness on van der Waals and electrostatic adhesion between a uniformly charged dielectric sphere and a grounded substrate. We find that roughness can either enhance or diminish the electrostatic contribution to adhesion depending on the particle size, permittivity and substrate morphology. Electrostatic forces become more prominent in the total adhesion force for larger particles. The effect of roughness on electrostatic adhesion is much less pronounced than that on van der Waals adhesion. As a result, roughness extends the particle size range where electrostatic forces are prominent.

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