A note on the effect of surface topography on adhesion of hard elastic rough bodies with low surface energy

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Abstract: Adhesion between bodies is strongly influenced by surface roughness. In this note, we try to clarify how the statistical properties of the contacting surfaces affect the adhesion under the assumption of long-range adhesive interactions. Specifically, we show that the adhesive interactions are influenced only by the roughness amplitude $h_{\text{rms}}$, while the rms surface gradient $h'_{\text{rms}}$ only affects the non-adhesive contact force. This is a remarkable result if one takes into account the intrinsic difficulty in defining $h'_{\text{rms}}$. Results are also corroborated by a comparison with self-consistent numerical calculations.

Keywords: Contact mechanics, adhesion, rough surface, contact stresses.

1 Introduction

Adhesion of surfaces is a widely investigated problem and is of fundamental importance in many fields of science, like biology [1], medicine [2, 3], and engineering [4]. The adhesion between rough surfaces is of practical interest both for elastic [5] and viscoelastic bodies [6, 7], as roughness alters the effective surface energy of contacting bodies.

For this reason, several researchers investigated the problem from both the experimental and theoretical point of views. Fuller and Tabor (FT), for example, elaborated the first model aimed at explaining the effect of roughness on adhesion [8]. They extended the Greenwood-Williamson (GW) asperity model [9] to the case of adhesion described with the Johnson, Kendall and Roberts (JKR) theory [10]. They found a surprising agreement with experiments, which showed roughness destroys adhesion reducing pull-off force. Moreover, they found that the pull-off force depends on a single parameter, "which may be regarded as representing the statistically averaged competition between the compressive forces exerted by the higher asperities trying to prise the surfaces apart and the adhesive forces between the lower asperities trying to hold the surfaces together" (Ref. [11]). However, this picture of adhesion is valid only when roughness has a single length scale, but roughness usually occurs on many different length scales. Moreover, the formalism used by Fuller and Tabor is fine if the area of real contact (and the adhesion force) is very small. For this reason, the FT theory received several criticisms [12, 13]. In particular, Pastewka and Robbins [13], comparing their fully numerical predictions of pull-off force with the Fuller and Tabor ones, found pull-off data very far from the FT predictions. However, such large deviation was partly due to effects of truncation in the tails of the heights distribution of their surfaces [14].

Persson with a completely different methodology based on a multiscale approach [15], found that small quantities of roughness can induce an increase in the effective interfacial energy as a result of the increase in the surface area. However, such effect is not observed when the adhesive contact of hard solids is investigated [16]. In this case and at sufficiently small wavelength, the JKR approach may become inappropriate, since the amplitude $\sigma$ of the sinusoid is comparable with the length scale $\varepsilon$ of the Lennard-Jones force law, and attractive tractions in the separation regions will then have a significant effect [17, 18]. In this limit, a DMT-type solution [19] may be preferred to a JKR one, as remarked already in Ref. [16, 20, 21].

The above picture witnesses the existence of an open debate in the scientific community on which effects roughness induces on adhesion of elastic surfaces.
In the present note, with the aid of an advanced multi-asperity model [20, 22], we try to shed light on this problem investigating the influence that some important roughness parameters have on the adhesion and, in particular, on the pull-off force. Our results do not give a definitive response to the initial question, but they put the attention on the effect that the mean square roughness amplitude \( h_{\text{rms}} \) and gradient \( h'_{\text{rms}} \) have on adhesion in a precise limit: the contact of hard solids with long-range adhesion interactions, where DMT-type models are known works quite well.

2 On the effect of mean square roughness amplitude \( h_{\text{rms}} \) and gradient \( h'_{\text{rms}} \) on pull-off force

Results are obtained with the Interacting and Coalescing Hertzian Asperities (ICHA) model [22, 23] where adhesion is modeled as suggested in Ref. [20]. For details of the formulation the reader is referred to these works. Here, we briefly recall that solution is obtained solving first the adhesiveless contact problem under the action of the force \( F_0 \). Then, according to the DMT hypothesis for which adhesive interactions do not alter the deformation of the bodies and act only outside the contact area, the effective contact force \( F_N \) producing the contact area \( A \) is calculated as difference between the non-adhesive (or repulsive) force \( F_0 \) and the adhesive one \( F_{ad} \)

\[
F_N = F_0 - F_{ad} = F_0 - \int_{A_{nc}} d^2 x p_a[u(x)]
\]

where \( A_{nc} \) is the non-contact area and \( p_a(u) \) is the adhesive force per unit area, whose value depends on the separation \( u \) between bodies, according to the equation (see Ref. [16, 19])

\[
p_a(u) = \frac{8w}{3d_c} \left[ \left( \frac{d_c}{u + d_c} \right)^9 - \left( \frac{d_c}{u + d_c} \right)^{3} \right]
\]

where \( w \) is the work of adhesion and \( d_c \) is the range of attractive forces of the order of the interatomic distance.

Notice, the adhesive force \( F_{ad} = \int_{A_{nc}} d^2 x p_a[u(x)] \) can be alternatively calculated as (see Ref. [16])

\[
F_{ad} = A_0 \int_0^\infty p_a(u)P(u)du
\]

where \( P(u) \) denotes the interfacial gap probability distribution, which is calculated by the solution of the adhesiveless contact problem, and \( A_0 \) is the nominal contact area.

Calculations are performed on self-affine fractal surfaces with power spectral density (PSD) assumed in a power law relation with the wave vector \( q = (q_x, q_y) \), with a constant value in a low wavenumber roll-off region

\[
C(q) = C_0 \quad \text{for } q_L \leq q < q_0
\]

\[
C(q) = C_0 \left( \frac{q}{q_0} \right)^{-2H+1} \quad \text{for } q_0 \leq q < q_1 \quad (4)
\]

and zero otherwise. Surfaces are numerically generated using the spectral methodology developed in Ref. [24, 25], and using \( q_L = 2.5 \cdot 10^5 \text{ m}^{-1} \), \( q_0 = 4q_L \), and \( q_1 = Nq_0 \), being \( N \) the number of scales. Two sets of simulations are considered. In the first one, surfaces have been generated by keeping constant the root mean square roughness amplitude \( h_{\text{rms}} \); in the second one, instead, we fixed the root mean square gradient \( h'_{\text{rms}} \). Adhesion energy \( w \), composite elastic modulus \( E^* \) and interatomic bond distance \( d_c \) have been assumed equal to 0.2 J/m², 1.33 \cdot 10^3 \text{ GPa} and 1 nm, respectively.

Fig. 1a shows the normalized contact area \( A/A_0 \) as a function of the dimensionless pressures \( \hat{F}_N = F_N/(A_0E^*) \), \( \hat{F}_0 = F_0/(A_0E^*) \), and \( \hat{F}_{ad} = F_{ad}/(A_0E^*) \) for different values of the rms gradient \( h'_{\text{rms}} \) and fixed \( h_{\text{rms}} = 0.52 \text{ nm} \). Fig. 1b shows, instead, the same type of plot for fixed \( h'_{\text{rms}} = 0.0026 \) and various values of \( h_{\text{rms}} \).

As expected, the dependence of the contact area on the repulsive load \( F_0 \) is practically linear and it is affected by \( h'_{\text{rms}} \) according to the known relation \( A/A_0 \approx 2F_0/(A_0E^*h'_{\text{rms}}) \), i.e., at fixed \( F_0 \), the relative contact area decreases as \( h'_{\text{rms}} \) increases. On the contrary, the surface rms gradient has no effect on the relation between contact area and adhesive force \( F_{ad} \). Indeed, in such case, all curves collapse in a single one. As a result, the dependence of the curves on \( h'_{\text{rms}} \) observed in Fig. 1a is exclusively due to the contribution of the repulsive interactions.

For the same reasons, Fig. 1b shows that the contribution of \( F_0 \) is not affected by \( h_{\text{rms}} \) and just a little increase in rms roughness amplitude is enough to strongly reduce the adhesion force.

Medina and Dini [26], investigating the adhesive contact between a rough elastic sphere and a rigid half-space, found that a very modest contact hysteresis appears for small roughness in the range where the DMT approach is widely believed to be valid. For this reason, in the framework of our model, it is reasonable neglecting hysteresis loss and assuming no change in the area-load curves during the loading and unloading phases. In micro- and nano-devices, for example, stickiness of contacting surfaces may represent an important problem and it can occur even when adhesive hysteresis is missing.

Under such hypothesis, the pull-off force, i.e., the force required to completely detach the surfaces, is the
Figure 1: The relative contact area $A/A_0$ as a function of the dimensionless applied pressures $\hat{F}_N$ (blue solid line), $\hat{F}_0$ (black dashed line), and $\hat{F}_ad$ (red dot-dashed lines) for (a) $h_{rms} = 0.52$ nm and different values of $h'_{rms} = 0.0011, 0.0014, 0.0016, 0.0026$; (b) $h'_{rms} = 0.0026$ and different $h_{rms} = 0.52$ nm, $0.68$ nm, $1.17$ nm.

Figure 2: The dimensionless pull-off pressure (taken as the modulus of the minimum value of the normalized applied pressure $\hat{F}_N$) as a function of the surface rms slope $h'_{rms}$. Results are shown for different values of the rms roughness amplitude $h_{rms}$. (b) Comparison of the predicted area vs. load results with the numerical GFMD data extracted from Figure 19 by Ref. [16].

2b further shows that such agreement concerns the whole curve relating the contact area and the applied load.

There is an intrinsic difficulty in defining the rms gradient, both on theoretical and practical levels. Indeed, the rms gradient is related to short wavelength components of the PSD spectrum. In particular, the value of $h_{rms}$ depends on the high cut-off frequency at which the truncation of the PSD spectrum is fixed. Real surfaces present very broad spectra, and roughness is characterized by several wavelengths from nano to micro scales. The choice of the cut-off frequency represents a critical step in modelling rough contacts. However, Solhjoo and Vakis [27] suggested that the limit of the high cut-off frequency can be identified via the PSD of relaxed atomic structures. They found $q_1 = 0.02$ nm$^{-1}$. Lorenz et al. [28] suggested that the truncation should occur where the rms gradient reaches $h_{rms} (q_1) = 1.3$, although there are no data available to interpret the generality of this recommendation. Other authors [29] suggested many factors could be associated to the truncation cut-off, including small dirt particles or rubber wear particles. From an experimental point of view, in practical cases, measurements of surface local gradient are closely related to instruments sensitivity [30]. Therefore, in view of this difficulty, the above results, showing independence of the pull-off force from the short wavelengths, are remarkable and are also in agreement with recent findings of Joe, Thouless and Barber [31] that showed the adhesive behavior of self-affine fractal surfaces is not
influenced by the high frequency cut-off (and hence by the smallest roughness structures).

3 Conclusions

In this work, we have shown that adhesive forces are influenced only by the rms roughness amplitude \( h_{\text{rms}} \), while repulsive interactions depend on the rms surface gradient \( h'_{\text{rms}} \). As a result, we have also found that the pull-off force is almost independent of \( h_{\text{rms}} \) in agreement with recent findings of other works of the literature. The present results apply in the limit of hard solids with long-range adhesive interactions and, consequently, the debate on which geometrical parameters affect the stickiness of randomly rough surfaces remains open.

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References

[1] Dening K., Heepe L., Afferrante L., Carbone G., Gorb S.N., Adhesion control by inflation: implications from biology to artificial attachment device, Appl. Phys. A, 2014, 116(2), 567-573.
[2] Lei W.S., Mittal K., Yu Z., Adhesion Measurement of Coatings on Biodevices/Implants: A Critical Review Reviews of Adhesion and Adhesives, 2016, 4(4), 367-397.
[3] de Tullio M.D., Afferrante L., Demelio G., Pascazio G., Verzicco R., Fluid-structure interaction of deformable aortic prostheses with a bileaflet mechanical valve, J. Biomech., 2011, 44(9), 1684-1690.
[4] Zhao Y.-P., Wang L.S., Yu T.X., Mechanics of adhesion in MEMS - a review, J. Adhesion Sci. Technol., 2003, 17(4), 519-546.
[5] https://doi.org/10.1163/1568561036054393
[6] Menga N., Afferrante L., Carbone G., Adhesive and adhesives contact mechanics of elastic layers on slightly wavy rigid substrates, Int. J. Solids Struct., 2016, 88, 101-109.
[7] Menga N., Afferrante L., Demelio G., Carbone G., Rough contact of sliding viscoelastic layers: numerical calculations and theoretical predictions, Tribol. Int., 2018, 122, 67-75.
[8] Menga N., Afferrante L., Carbone G., Effect of thickness and boundary conditions on the behavior of viscoelastic layers in sliding contact with wavy profiles, J. Mech. Phys. Solids, 2016, 95, 517-529.
[9] Fuller K.N.G., Tabor D., The Effect of Surface Roughness on the Adhesion of Elastic Solids, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 1975 345(1642), 327-342.
[10] Greenwood J. A., Williamson J.B.P., Contact of Nominally Flat Surfaces. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 1966, 295(1442), 300-319.
[11] Johnson K.L., Kendall K., Roberts A.D., Surface Energy and the Contact of Elastic Solids, Proc. Royal Soc. A: Math., Phys. Eng. Sci., 1971 324(1558), 301-313.
[12] Persson B.N.J., Tosatti E., The effect of surface roughness on the adhesion of elastic solids, J. Chem. Phys., 2001, 115(12), 5597-5610.
[13] Pastorino R., Robbins M.O., Contact between rough surfaces and a criterion for macroscopic adhesion, Proc. Nat. Acad. Sci., 2014, 111(9), 3298–3303.
[14] Ciavarella M., Papangelo A., Afferrante L., Adhesion between self-affine rough surfaces: Possible large effects in small deviations from the nominally Gaussian case, Tribol. Int., 2017, 109, 435-440.
[15] Persson B.N.J., Adhesion between an elastic body and a randomly rough hard surface, Eur. Phys. J. E 2002, 8, 385-401.
[16] Persson B.N.J., Scaraggi M., Theory of adhesion: Role of surface roughness, J. Chem. Phys., 2014, 141(12), 124701.
[17] Afferrante L., Ciavarella M., Demelio G., Adhesive contact of the Weierstrass profile, Proc. Royal Soc. A: Math. Phys. Eng. Sci., 2015, 471(2182), 20150248.
[18] Ciavarella M., Afferrante L., Adhesion of rigid rough contacts with bounded distribution of heights, Tribol. Int., 2016, 100, 18-23.
[19] Muller V.M., Derjaguin B.V., Toporov Y.P., On two methods of calculation of the force of sticking of an elastic sphere to a rigid plane, Colloids Surf., 1983, 7(3), 251-259.
[20] Violano G., Afferrante L., On DMT methods to calculate adhesion in rough contacts, Tribol. Int., 2019, 130, 36-42.
[21] Violano G., Afferrante L., Contact of rough surfaces: Modeling adhesion in advanced multiscaleity models, Proc. Instit. Mech. Eng, Part J: J. Eng. Tribol., 2019 https://doi.org/10.1177/1350650119838669
[22] Afferrante L., Carbone G., Demelio G., Interacting and coalescing Hertzian asperities: A new multiscaleity contact model, Wear, 2012, 278-279, 28-33.
[23] Afferrante L., Bottiglione F., Putignano C., Persson B.N.J., Carbone G., Elastic contact mechanics of randomly rough surfaces: an assessment of advanced asperity models and Persson’s theory, Tribol. Lett., 2018, 66, 75.
[24] Putignano C., Afferrante L., Carbone G., Demelio G., A new efficient numerical method for contact mechanics of rough surfaces, Int. J. Solids Struct., 2012, 49(2), 338-343.
[25] Putignano C., Afferrante L., Carbone G., Demelio G., The influence of the statistical properties of self-affine surfaces in elastic contacts: A numerical investigation, J. Mech. Phys. Solids, 2012, 60(5), 973-982.
[26] Medina S., Dini D., A numerical model for the deterministic analysis of adhesive rough contacts down to the nanoscale, Int. J. Solids Struct., 2014, 51(14), 2620-2632.
[27] Soljic D., Stojčić S., Vakis A.I., Surface roughness of gold substrates at the nanoscale: An atomistic simulation study, Tribol. Int., 2017, 115, 165-178.
[28] Lorenz B., Oh Y.R., Nam S.K., Jeon S.H., Persson B.N.J., Rubber friction on road surfaces: Experiment and theory for low sliding speeds, J. Chem Phys., 2015, 142(19), 194701.
[29] Carbone G., Putignano C., Rough viscoelastic sliding contact: theory and experiments, Phys. Rev. E, 2014, 89(3), 032408.
[30] Persson, B. N. J. (2014). On the fractal dimension of rough surfaces. Tribology Letters, 54(1), 99-106. https://doi.org/10.1007/s11249-014-0313-4
[31] Joe J., Thouless M.D., Barber J.R., Effect of roughness on the adhesive tractions between contacting bodies, J. Mech. Phys. Solids, 2018, 118, 365-373.