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Influence of self-affine roughness on the detachment stress at an elastic-inelastic interface

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This work concentrates on the influence of roughness on the detachment stress of an elastic body in contact to self-affine rough surfaces. It is shown that the self-affine roughness influences the detachment stress depending on the elastic modulus E and the details of the specific roughness. The roughness influence is more dominant for detachment lengths λ smaller or comparable to the in-plane roughness correlation length ξ, and low roughness exponents H (<0.5). The detachment stress as a function of the correlation length ξ shows a maximum for correlation lengths $\xi>\lambda$ and low roughness exponents $(H<0.5)$, while the correlation length ξ where the maximum occurs approaches the size of the detachment length λ with increasing roughness exponent H.

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I. INTRODUCTION

The adhesion of elastic bodies onto hard solid substrates is influenced by the presence of surface roughness, which has important consequences from both a fundamental and technological point of view in various applications, e.g., polymer/metal junctions. This topic was studied initially by Fuller and Tabor,[1] showing that a relatively small surface roughness could not only diminish but also remove the adhesion. In this work the authors applied the contact theory by Johnson *et al.*[2] for each individual asperity, and it was considered a Gaussian distribution of asperity heights with all asperities having the same radius of curvature.

On the other hand, random rough surfaces, which are commonly encountered for solid surfaces,[3,4] have roughness over different length scales rather than a single one. This case was considered by Persson and Tosatti[5] for the case of random self-affine rough surfaces. It was shown that when the local fractal dimension D is larger than 2.5 the adhesive force may vanish or at least be reduced significantly. Since $D=3-H$ with H the roughness exponent, which characterizes the degree of surface irregularity (as H becomes smaller the surface becomes more irregular at short length scales), the roughness effect becomes more prominent for roughness exponents $H<0.5$ $(D>2.5)$.[5]

Furthermore, it has been shown that the self-affine roughness at the junction of an elastic film and a hard solid substrate influences its detachment force in a way that it can be smaller than that of a flat surface, depending also on the specific roughness details.[6] For rougher surfaces, the effect of elastic energy becomes more dominant with an increasing ratio between the roughness amplitude w and the roughness correlation length ξ along the interface. The detachment force showed a maximum after which it decreased and became even lower than that of a flat surface.[6]

The detachment of an elastic body from a rough solid interface does not occur at once but by the formation of cracks along the interface leading to stress distributions which strongly depend on the particular surface morphology. In this paper, we will investigate properties of the detachment stress by taking into account the specific roughness characteristics not only for roughness wavelengths less than ξ (probing only the power-law regime), but also including contributions from roughness wavelengths greater than ξ.

II. BASIC THEORY CONCEPTS

In the following we assume an elastic film of elastic modulus E and Poisson's ratio ν on top of a rough substrate. The substrate surface roughness is described by the single-valued random roughness fluctuation function $h(r)$ with r the in-plane position vector $r=(x,y)$ such that $\langle h(r)\rangle=0$. Furthermore, we consider the system on the characteristic length scale λ assigned to describe the size of the detachment length. The stress $\sigma_d(\lambda)$ necessary to induce a detached area of width λ can be obtained from that of a penny-shaped crack of diameter λ and it is given[7,8]

$$\sigma_d(\lambda)=\left[\frac{\pi E}{1-\nu^2}\,\frac{\Delta\gamma_{\mathrm{eff}}(\lambda)}{\lambda}\right]^{1/2}, \tag{1}$$

where $\Delta\gamma_{\mathrm{eff}}$ is the effective change in surface energy due to substrate roughness. The derivation of Eq. (1) can be easily understood as follows. Creation of an interfacial crack of width λ requires a surface energy $\approx\Delta\gamma_{\mathrm{eff}}\lambda$ per unit of the crack line length, while the crack formation lowers the linear elastic energy in an area proportional to λ^2 from the value $\approx\sigma_d^2(\lambda)/E$ before detachment to almost 0 after detachment.[7] If we minimize the total energy $\Delta\gamma_{\mathrm{eff}}\lambda-\lambda^2\,\sigma_d^2(\lambda)/E$ we obtain qualitatively $\sigma_d(\lambda)=[2E\Delta\gamma_{\mathrm{eff}}(\lambda)/3\lambda]^{1/2}$, where a more exact calculation gives Eq. (1).[8]

The quantity $\Delta\gamma_{\mathrm{eff}}$ is obtained by the total free energy of the elastic film[5]

$$\Delta\gamma_{\mathrm{eff}}=-[U_{\mathrm{ad}}+U_{\mathrm{el}}]/A_{\mathrm{flat}}, \tag{2}$$

$$U_{\mathrm{ad}}=-\Delta\gamma A_{\mathrm{flat}}\int_0^{+\infty}\sqrt{(1+\rho_\lambda^2 u)}\,e^{-u}du,$$

$$U_{\mathrm{el}}=A_{\mathrm{flat}}\;\frac{E}{4(1-\nu^2)}\int_{Q_\lambda}^{Q_c}qC(q)d^2q, \tag{3}$$

where U_{ad} is the adhesive energy and U_{el} is the elastic energy stored in the film. $-\Delta\gamma$ is the change of the local surface free energy upon contact due to elastic body and substrate interaction. In fact, for an interface between dissimilar materials E and ν in Eq. (3) correspond to the parameters of the two separate elastic media via the relationship $(1-\nu^2)/E=\Sigma_{i=1,2}(1-\nu_i^2)/E_i$. Here we assume that there is no substantial elastic energy stored in the hard substrate but only in the compliant layer on top with a modulus E. The local surface slope ρ_λ is given by[7]

$$\rho_\lambda=\left[\int_{Q_\lambda}^{Q_c} q^2 C(q) d^2 q\right]^{1/2}. \tag{4}$$

For the elastic energy stored in the film we assume that the normal displacement field of the film equals $h(r)$.[5] $C(q)$ is the Fourier transform of the substrate height-height correlation function $C(r)=\langle h(r)h(0)\rangle$ that characterizes the substrate roughness, and $Q_c=\pi/a_o$ with a_o of the order of atomic dimensions.

III. RESULTS AND DISCUSSION

Calculations of the detachment stress require knowledge of the roughness spectrum $C(q)$. For the self-affine surface roughness $C(q)$ scales as a power-law $C(q)\propto q^{-2-2H}$ if $q\xi \gg 1$, and $C(q)\propto \mathrm{const}$ if $q\xi \ll 1$.[3,4] The roughness exponent H is a measure of the degree of surface irregularity,[3,4] such that small values of H characterize more jagged or irregular surfaces at short length scales ($<\xi$). This scaling behavior is satisfied with a simple Lorentzian form[9]

$$C(q)=\frac{1}{2\pi}\frac{w^2\xi^2}{(1+aq^2\xi^2)^{1+H}} \tag{5}$$

with $a=(1/2H)[1-(1+aQ_c^2\xi^2)^{-H}]$ if $0<H<1$. For other correlation models see also Refs. 4 and 10. Calculations of the local surface slope from Eq. (5) yields

$$\rho_\lambda=\frac{w}{\sqrt{3}a\xi}\left[\frac{1}{1-H}\{T_c^{1-H}-T_\lambda^{1-H}\}+\frac{1}{H}\{T_c^{-H}-T_\lambda^{-H}\}\right]^{1/2} \tag{6}$$

with $Q_\lambda=2\pi/\lambda$, $T_\lambda=(1+aQ_\lambda^2\xi^2)$, and $T_c=(1+aQ_c^2\xi^2)$. Furthermore, for the elastic energy U_{el} we have an analytic expression for exponents $H=0$, $H=0.5$, and $H=1$. Indeed, if we set $w_o=\sqrt{4(1-\nu^2)/E}$ we have

$$U_{\mathrm{el}}|_{H=0}=A_{\mathrm{flat}}\ \frac{w^2}{w_o^2}\left\{\frac{1}{a}(Q_c-Q_\lambda)-\frac{1}{a^{3/2}\xi}[\tan^{-1}(X_c)-\tan^{-1}(X_\lambda)]\right\}, \tag{7}$$

$$U_{\mathrm{el}}|_{H=0.5}=A_{\mathrm{flat}}\ \frac{w^2}{w_o^2}\left\{\frac{1}{a^{3/2}\xi}[\sinh^{-1}(X_c)-\sinh^{-1}(X_\lambda)]-\frac{1}{a}-[Q_cT_c^{-1/2}-Q_\lambda T_\lambda^{-1/2}]\right\}, \tag{8}$$

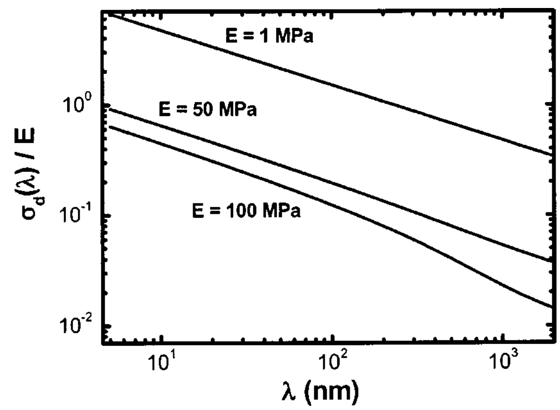

FIG. 1. Detachment stress $\sigma_d(\lambda)$ versus detachment length λ for various elastic moduli E, $H=0.7$, $w=10$ nm, and $\xi=200$ nm.

$$U_{\mathrm{el}}|_{H=1}=A_{\mathrm{flat}}\ \frac{w^2}{w_o^2}\left\{\frac{1}{a^{3/2}\xi}[\tan^{-1}(X_c)-\tan^{-1}(X_\lambda)]-\frac{1}{2a}[Q_cT_c^{-1}-Q_\lambda T_\lambda^{-1}]\right\}, \tag{9}$$

with $X_c=\sqrt{a}\xi Q_c$ and $X_\lambda=\sqrt{a}\xi Q_\lambda$.

In the following the calculations were performed for relatively small roughness amplitudes so that $w/\xi<0.1$, $w=10$ nm, Poisson's ratio $\nu=0.4$, and change in surface energy (in the absence of roughness) $\Delta\gamma=3$ meV/Å^2, typical for a polymer-metal interface. With increasing elastic modulus E as is shown in Fig. 1 the stress $\sigma_d(\lambda)$ decreases with respect to E since the storage of elastic energy favors easier detachment of the elastic body. Furthermore, since $C(q)\propto w^2$, the influence of the rms roughness amplitude w on the stress $\sigma_d(\lambda)$ is rather simple ($\sigma_d\propto w$), while any complex dependence will arise solely from the roughness parameters H and ξ (or the ratio w/ξ).

As Fig. 2 indicates with decreasing roughness exponent H, the detachment stress $\sigma_d(\lambda)$ increases significantly especially for small detachment lengths λ ($<\xi$). This is because the lower the roughness exponent H the larger is the surface area and thus the adhesive energy. However, the stress $\sigma_d(\lambda)$

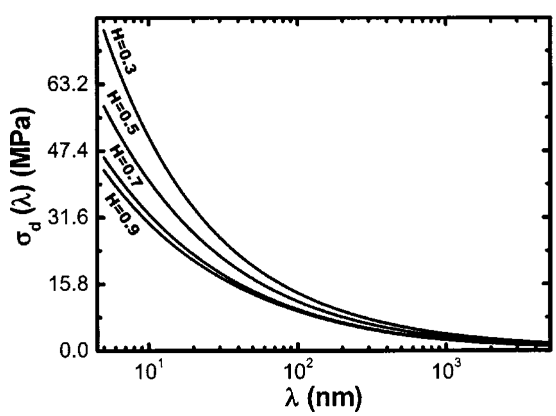

FIG. 2. Detachment stress $\sigma_d(\lambda)$ versus detachment length λ for various roughness exponents H, $E=50$ MPa, $w=10$ nm, and $\xi=200$ nm.

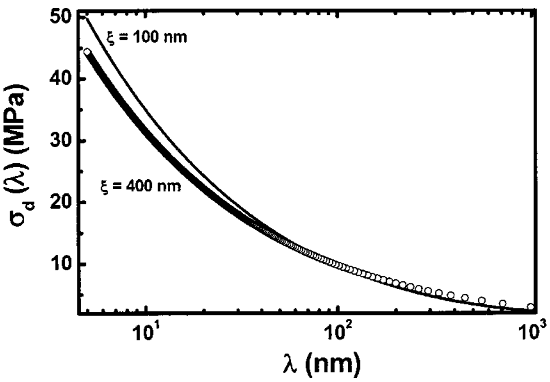

FIG. 3. Detachment stress $\sigma_d(\lambda)$ versus detachment length λ for various roughness correlation lengths ξ, $H=0.7$, $E=50$ MPa, $w=10$ nm.

shows the opposite behavior with increasing correlation at large length scales λ as Fig. 3 shows, which is due to the competition of elastic and adhesive energy terms. For short detachment lengths $\lambda<\xi$ a rougher surface (smaller H and/or larger ratio w/ξ) will lead to higher detachment stress.

In order to gauge more precisely the effect of the roughness parameters H and ξ we plot in Fig. 4 the detachment stress $\sigma_d(\lambda)$ as a function of the roughness correlation length ξ for various roughness exponents H. As can be seen from Fig. 4, the stress $\sigma_d(\lambda)$ has a maximum at a correlation length $\xi>\lambda$, which shifts towards the value $\xi\approx\lambda$ as the roughness exponent H increases and becomes larger than 0.5. The maximum is more pronounced for small roughness exponents ($H<0.5$), and it is clear that the detachment stress has a multivalued behavior around the maximum. The shape of the maximum is not only affected by the elastic modulus E and the roughness exponent H, but also by the value of the lateral correlation length ξ or alternatively the ratio w/ξ. Indeed, Fig. 4 shows that upon smoothening of the surface the maximum broadens, preceded by a faster change of the detachment stress as a function the contact length λ.

Moreover, as Fig. 5 shows, the maximum is more pronounced for higher elastic modulus values E. For low elastic modulus E so that $U_{\mathrm{ad}}\gg U_{\mathrm{el}}$ the detachment stress decreases

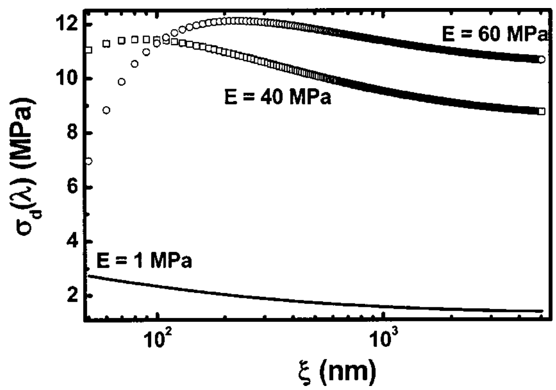

FIG. 5. Detachment stress $\sigma_d(\lambda)$ versus correlation length ξ for detachment length $\lambda=100$ nm, various elastic moduli E, $H=0.5$, and $w=10$ nm.

with increasing roughness correlation ξ or by roughness smoothing since the surface area and thus the adhesive term decreases (see in Fig. 5 the curve for $E=1$ MPa). If the elastic modulus E decreases during the detachment process, which involves pulling-off of the attached body on the rough solid substrate, the detachment stress will be drastically reduced. In fact, in the case of a high molecular weight monodisperse polymers it is interesting to note that the elastic modulus varies with time and the energy of adhesion depends on the time of contact.[11]

It is thought to decrease for short time scales (say, i.e., $t<\tau_c$) first, approximately according to a power law. It becomes constant till a time τ_d, after which it decreases again according to viscous flow. To incorporate the time dependence, calculations were performed for $H=0.5$, $w=10$ nm, and $\tau_c=0.005$ s and a time-dependent modulus described by the relation $E(t)=(E_o/e)\exp(\sqrt{\tau/\tau_c})$ $(\tau\leqslant\tau_c)$ with $E_o=100$ MPa. The results are displayed in Fig. 6, where it is shown clearly as the elastic modulus decreases with time the effect of the elastic term diminishes substantially as it is explained previously.

IV. CONCLUSIONS

This work concentrates on the influence of roughness on the detachment stress of an elastic bobby in contact onto a

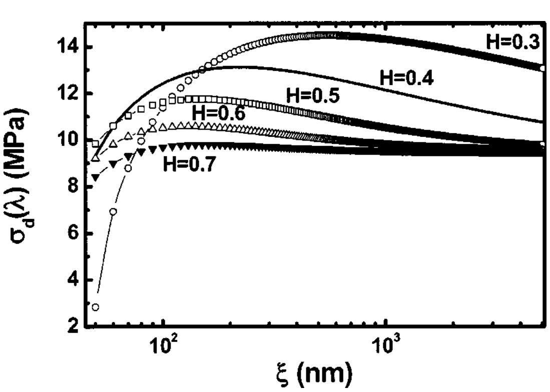

FIG. 4. Detachment stress $\sigma_d(\lambda)$ versus correlation length ξ for detachment length $\lambda=100$ nm, various roughness exponents H, $E=50$ MPa, and $w=10$ nm.

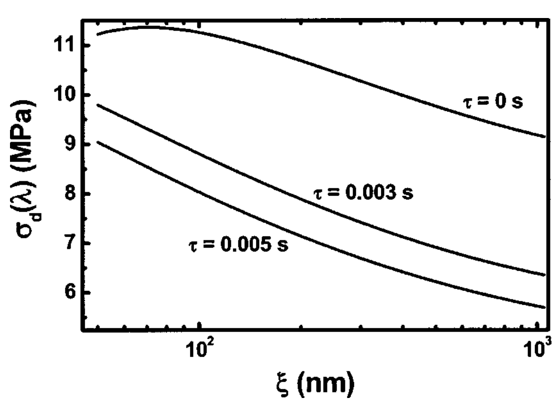

FIG. 6. Detachment stress $\sigma_d(\lambda)$ versus correlation length ξ for detachment length $\lambda=100$ nm, various times τ, $H=0.5$, and $w=10$ nm.

self-affine rough surface. It is shown that the self-affine roughness influences the detachment stress in a manner that depends on the elastic modulus E and the details of the specific roughness. The roughness influence is more dominant for detachment lengths λ smaller than or comparable to the in-plane roughness correlation length ξ and low roughness exponents H (<0.5). The detachment stress as a function of the correlation length ξ shows a maximum for correlation lengths $\xi>\lambda$ and low roughness exponents ($H<0.5$), while the correlation length ξ where the maximum occurs approaches the size of the detachment length λ with increasing roughness exponent H.

The multivalued behavior around the maximum further complicates the influence of the roughness. These results clearly indicate that the substrate roughness has to be precisely quantified in detachment experiments. However, we should note that our analytic calculations are strictly valid for elastic solids, while for real, e.g. polymers[11–13] time-dependent elastic effects are present which also alter, besides the precise value for the elastic modulus E, the value of change in surface energy $\Delta\gamma$, which is considered here in the adiabatic limit. In this case surface roughness introduces fluctuating forces with a wide distribution of frequencies.[12]

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