Roughness effects on the electrostatic-image potential near a dielectric interface

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In this work, we investigate roughness effects on the electrostatic-image potential of a point charge situated in the vicinity of a rough dielectric–vacuum interface. The roughness is modeled as a self-affine structure with root mean square roughness $\sigma$, correlation length $\xi$, and roughness exponent $0<H<1$. The roughness contribution on the electrostatic-image potential could be significantly large (>$10\%$) with respect to that of a flat interface, and its effect outside the dielectric medium is dominated mainly by the long-wavelength roughness parameters $\sigma$ and $\xi$. However, inside the medium, the contribution of the roughness exponent $H$ could become comparable to that of $\sigma$ and $\xi$. © 1997 American Institute of Physics. [S0021-8979(97)02513-9]

I. INTRODUCTION

The notion of the image potential is encountered in a wide variety of physical systems whenever a charged particle is located in the vicinity of a solid surface under conditions where the solid can be considered as a continuum medium. Examples include the binding of electrons near the surface of liquid He due to the potential well formed by the long-range repulsive potential, the motion of electrons above solid–liquid He due to the potential well formed by the long-range repulsive potential, and the short-range electron-atom interaction. The motion of electrons above solid surfaces where electron-surface plasmon scattering events (proving the extension of the plasmon potential out of the solid surface) occur, the shifting of the electron energy levels in the inversion layer at a semiconductor–oxide interface etc.

If the solid is characterized by an isotropic dielectric tensor, the electrostatic potential of such a composite system can be expressed as a sum of the direct point charge Coulomb potential, and the potential (image potential) of a fictitious charge located at the position of the image (reflection) of the true charge with respect to the dielectric–vacuum interface. The concept of the image potential can be generalized to the case of a nonplanar (curved) interface, and to an interface that separates two different dielectric media each of which is described by an anisotropic dielectric tensor.

In most of the cases where image-potential effects have been considered, the interface between dielectric–vacuum (or dielectric–dielectric) was assumed to be planar. However, real surfaces have always some degree of imperfection (roughness) which depends on the method of surface treatment, the growth conditions, and the particular material. Therefore, it is necessary and interesting to examine the extent to which the image potential is influenced by possible morphological imperfections, and in turn to determine their implications on physical systems where the concept of the electrostatic-image potential is considered.

Up to now a quantitative analysis of surface roughness effects on the image potential was mainly performed for the case of random Gaussian roughness which was described by the correlation function $C(r) = \sigma^2 e^{-(r/\xi)^2}$ with $\sigma$ the rms roughness, and $\xi$ the in-plane roughness correlation length. It was shown that surface roughness yields on the image potential were as high as even $10\%$–$60\%$ compared to that of a flat interface, depending mainly on the relative magnitude of the roughness correlation length $\xi$ with respect to the distance of the image charge to the point where the potential was determined. However, the roughness effects on the electrostatic potential were not investigated in detail inside the dielectric medium and compared to that outside the medium. The previously studied morphology effects cannot account for rough surfaces grown under conditions far from equilibrium, and those characterized in many instances by self-affine scaling.

In the latter case, the surface morphology is characterized, apart from the roughness parameters $\sigma$ and $\xi$, by an additional component at small length scales which is the degree of surface irregularity. The latter is described by a roughness exponent $H$ ($0<H<1$) which is also associated with a local fractal dimension $D_H = 3 - H$.

Therefore, an investigation is in order of the impact of the interface irregularity described by the exponent $H$, and in comparison with that of the other roughness parameters $\sigma$ and $\xi$, on the electrostatic potential of the composite system point charge dielectric. Furthermore, a detailed extension of the previous studies of the roughness effect in all regions of space will be performed in order to achieve a more complete knowledge and understanding of surface/interface roughness on the electrical properties of matter. Particular emphasis will be given to morphology effects arising from nanoscale roughness characteristics, since modern fabrication techniques, e.g., molecular beam epitaxy (MBE), allow the formation of high quality surfaces and interfaces.

II. ELECTROSTATIC POTENTIAL AND POISSON EQUATION

The electrostatic-image potential will be calculated for an isotropic medium of dielectric constant $\varepsilon$ occupying the half-space ($z<0$) terminated to an interface with a profile $z = h(r)$, and a point charge $q$ situated in vacuum at the origin.

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position \((\mathbf{r}', z')\). The profile function \(z = h(\mathbf{r})\) \((h(\mathbf{r}) = 0)\) is assumed to be a stationary stochastic function of the in-plane position vector \(\mathbf{r} = (x, y)\). The electrostatic potential \(\Phi = \Phi(\mathbf{r}, z, \mathbf{r}', z')\) at a point \((\mathbf{r}, z)\) is a solution of the Poisson equation\(^1\)

\[ \nabla^2 \Phi = \begin{cases} -4\pi \rho \delta(z-z') \delta^2(\mathbf{r}-\mathbf{r}'), & z > h(\mathbf{r}) \\ 0 & z < h(\mathbf{r}) \end{cases}, \]  

under the boundary conditions

\[ \Phi \big|_{z=h(\mathbf{r})^-} = \Phi \big|_{z=h(\mathbf{r})^+}, \]  

\[ \epsilon \mathbf{n} \cdot \nabla \Phi \big|_{z=h(\mathbf{r})^-} = -\nabla \Phi \big|_{z=h(\mathbf{r})^+}, \]  

with \(\mathbf{n} = (-\partial h/\partial x, -\partial h/\partial y, 1)[1 + (\nabla h)^2]^{-1/2}\) the unit vector normal to the surface. The general solution of Eq. (1) can be written in the form\(^4\)

\[
\Phi = \begin{cases} \int \frac{d^2k}{(2\pi)^2} \frac{2\pi q}{k} e^{ik(\mathbf{r}-\mathbf{r}')-k|z-z'|} + \int \frac{d^2k}{(2\pi)^2} A(k)e^{ikr-kz}, & z > h(\mathbf{r}) \\ 0 & z < h(\mathbf{r}) \end{cases},
\]

The first term in Eq. (3) for \(z > h(\mathbf{r})\) is the particular integral of Eq. (1), while the remaining terms are solutions of the corresponding homogeneous Poisson equation.

The coefficients \(A(k)\) and \(B(k)\) in Eq. (3) are determined in a perturbative manner (see the Appendix) for the case of weak roughness \(|\nabla h| \ll 1\). Substitution of \(\Phi\) into Eq. (3) and ensemble averaging over roughness realizations, assuming the roughness to be statistically stationary up to second order \(\langle h(\mathbf{k})h^*(\mathbf{k}')\rangle = (2\pi)^2\delta(\mathbf{k}+\mathbf{k}')\langle |h(\mathbf{k})|^2\rangle\), we obtain

\[
\Phi = \int \frac{d^2k}{(2\pi)^2} \frac{q(\epsilon-1)}{\xi(p^2+s^2)^{1/2}} + \Phi_2^r(s,p) \quad (z > 0 \text{ and } z' > 0),
\]

\[
\Phi = \frac{2q}{(\epsilon+1)\xi(p^2+s^2)^{1/2}} \Phi_2^0(s,p) \quad (z < 0 \text{ and } z' > 0),
\]

\[
\Phi_1^r(s,p) = \frac{-q(\epsilon-1)}{2\pi^2(\epsilon+1)^2} \int_0^{Q_0<k<\kappa} \int_0^\pi \langle |h(\mathbf{k}-\mathbf{Q})|^2 \rangle kQ^2J_0(kp\xi)D_{1,2}(\theta) e^{-s\frac{kQ^2}{2}} dk dQ d\theta,
\]

with \(D_1(\theta) = \epsilon(\epsilon-1) + 4\epsilon \cos \theta - (\epsilon-1)\cos^2 \theta, D_2(\theta) = (\epsilon-1)[2\cos \theta - \cos^2 \theta - 1], J_0(x)\) the zero order Bessel function, and \(|\mathbf{k}-\mathbf{Q}| = (k^2+Q^2-2kQ \cos \theta)^{1/2}\). Moreover, we have defined the parameters \(d = |z-z'|/\xi, \quad p = |\mathbf{r}-\mathbf{r}'|/\xi, \quad s = (|z|+|z'|)/\xi, \quad \kappa = \pi/a_0\) is an upper cutoff with \(a_0\) to the order of the atomic spacing.

The first term in Eq. (4) \(\Phi_2^r(s,p)\) represents the electrostatic potential from a flat surface \((\Phi_2^r,s,p)\), and the second term \(\Phi_1^r(s,p)\) is the contribution due to roughness to the order \(O(\sigma^2/\xi^3)\). We point out that the ensemble average over roughness realizations restores infinitesimal translation invariance in such a way that the ensemble averaged potential will depend only on the reference \(|\mathbf{r}-\mathbf{r}'|\). 

III. ELECTROSTATIC POTENTIAL FOR SELF-AFFINE MORPHOLOGY

A wide variety of surfaces and interfaces occurring in nature is well represented by a kind of roughness associated with self-affine fractal scaling, \(^6\) defined by Mandelbrot in terms of fractional Brownian motion. \(^7\) Examples include the nanometer topology of vapor-deposited thin films, the spatial fluctuations of liquid–gas interfaces, the kilometer-scale structure of a mountain terrain, etc. \(^6\) Physical processes that produce such surfaces include fracture, erosion, MBE, and fluid invasion in porous media to name several. \(^6\)

The correlation function \(C(r) = \langle h(\mathbf{r})h(0)\rangle\) for any physical isotropic self-affine surface scales as \(C(r) \sim \sigma^2 e^{-D_{1/2}r^H}\) for \(r \ll \xi\), and \(C(r) = 0\) for \(r \gg \xi\) \((D = 3\sigma^2/\xi^2\) is a constant). \(^6\) The Fourier transform of \(C(r)\), \(\langle |h(\mathbf{r})|^2 \rangle\), scales as \(\langle |h(\mathbf{k})|^2 \rangle \sim k^{-2-2H}\) if \(k\xi > 1\), and \(\langle |h(\mathbf{k})|^2 \rangle \sim \text{const}\) if \(k\xi < 1\) \(^9\). This scaling behavior is satisfied by the simple correlation model, \(^9\)

\[
\langle |h(\mathbf{k})|^2 \rangle = (2\pi)^2 \frac{\sigma^2 \xi^2}{1+a(k^2+\xi^2)^{H}},
\]

for roughness exponents \(0 < H < 1\). The parameter \(\sigma^2\) is given by \(\sigma = (1/2H)\left[1 - (1+k^2\xi^2)^{-H}\right]\), if \(0 < H < 1\), and \(\sigma = (1/2)\ln(1+k^2\xi^2)\) if \(H = 0\). The limiting case of \(H = 0\) corresponds to logarithmic roughness. \(^9\) Moreover, for \(H = 0.5\) and \(\xi > a_0\) \((a \approx 1)\), Eq. (6) yields the simple exponential correlation \(C(r) \sim e^{-r^2/\xi^2}\). \(^9\) The Gaussian correlation \(C(r) = \sigma e^{-r^2/\xi^2}\) \((\text{Ref. 10})\) for \(H = 1\), while the exponential for \(H = 0.5\) \(9\)
We will limit ourselves to the simple but important case of $p=0$ ($|r-r'|=0$) where the roughness contribution is maximum since $J_0(0) = 1$. In fact, this case arises in a variety of physical systems, e.g., electron energy levels in the inversion layer at a semiconductor–oxide interface, and binding potential of electrons near a liquid He surface. From Eqs. (5) and (6) we obtain

$$
\Phi_r^{1,2}(s) = \frac{q(e-1)c^2}{\pi(e+1)^2} \times \int_0^{\infty} \int_0^{k_Q} \frac{\xi^2 \kappa \Omega(k,\Omega) e^{-\xi k}}{(1 + a \xi \Omega + a \xi^2 k^2)^{1-H} d \Omega d k},
$$

Equation (7) shows that the complex dependence of the roughness contribution $\Phi_r^{1,2}$ on the morphology characteristics comes solely from the parameters $H$ and $\xi$, while the rms roughness yields only a trivial dependence $\Phi_r^{1,2} \propto \sigma^2$.

**IV. RESULTS AND DISCUSSION**

Prior to the presentation of the results, we wish to point out that the ratio $\sigma/\xi$ describes mainly the long-wavelength ($r>\xi$) roughness characteristics, while finer roughness details at short wavelengths ($r<\xi$) are revealed through the effect of the roughness exponent $H$ which describes the degree of surface irregularity. In our calculations, we used values for the rms roughness $\sigma$ and correlation length $\xi$ such that $\sigma/\xi < 0.5$ in accordance with experimental observations over a wide variety of rough morphologies, and roughness exponents in the range $0 < H < 1$. Finally, since modern fabrication techniques (e.g., MBE) allow the formation of high quality interfaces, we will focus mainly on morphology effects arising from nanoscale roughness at an atomic level (e.g., $\sigma = a_0$).

Figure 2 depicts the variation of $|\Phi_r^1|/\Phi_{flat}^1$ as a function of the parameter $s = (|z| + |z'|)/\xi$ for two extreme values of the roughness exponent $H$. The effect of the latter is rather negligible ($<2\%$) with respect to that of the parameter $s$ which yields a rapid exponential decay of $\Phi_r^1$. By contrast, the effect of the roughness exponent $H$ is significantly pronounced for the electrostatic potential inside the medium $\Phi_r^1$ as can be seen in Fig. 3. As the roughness exponent $H$ spans the range from 0 to 1, $|\Phi_r^1|/\Phi_{flat}^1$ decreases even more than 10% which is comparable in magnitude with the effect of the parameter $s$ over the entire range of $s$ values. Moreover, $\Phi_r^1$ shows a weak extremum behavior for small $s (<0.5)$ which is enhanced as the roughness exponent increases towards large values ($H>1$). Therefore, although the absolute magnitude of the roughness contribution outside the medium for small $s (<1)$ is significantly larger than that inside, the latter shows a pronounced sensitivity to short-wavelength roughness details that pertain even for large values of the relative distance $s$ (or $|z| + |z'| > \xi$).

Figure 3 shows $|\Phi_r^1|/\Phi_{flat}^1$ vs $s$ where the effect of the roughness exponent $H$ appears more evident at large correlation lengths $\xi$ ($\sigma/\xi < 0.05$) in such a way that as $H$ decreases the roughness contribution increases. The inset of Fig. 4 shows that the roughness exponent $H$ accounts for a contribution of...
less than 5%, which, however, is significantly weaker (even by an order of magnitude) in comparison with that of $\xi$ and $s$. Thus the contribution of interface roughness to the image potential and subsequently to the electrostatic potential outside of the dielectric medium is dominated mainly by the long-wavelength roughness features ($\sigma, \xi$), and the distance of the image charge to the point where the potential is determined relative to the roughness correlation length.

In the following, we will examine the roughness contribution to the electrostatic potential inside the dielectric medium ($\Phi_r^2$) as a function of $H$ and $\xi$. Figure 5 depicts $|\Phi_r^2|/\Phi_{\text{flat}}^2$ vs $\xi$ where a distinct behavior unlike that of $\Phi_f^2$ in Fig. 4 is observed. Although the roughness contribution is remarkably smaller than that in the exterior of the medium, the effect of the roughness exponent $H$ is significantly more pronounced and is characterized by a rapid decrement of $|\Phi_r^2|/\Phi_{\text{flat}}^2$ at small $H$ ($<0.5$). Therefore if we compare the relative evolution of $\Phi_r^2/\Phi_{\text{flat}}^2$ as a function of $H$ and $\xi$, respectively, we can infer that the contribution by both roughness parameters is comparable in magnitude ($\sim 10\%$). Therefore, interface roughness contributes significantly to the electrostatic potential inside the dielectric medium over the entire range of roughness wavelengths described by the parameters $H$ (short wavelength), and $\sigma/\xi$ (long wavelengths).

From what we have discussed, we can infer that the roughness contribution $\Phi_r^{1,2}$ as a function of the roughness exponent $H$ has, in general, an upper bound such that $|\Phi_r^{1,2}|_{H=\varepsilon}<|\Phi_r^{1,2}|_{H=0}$ if $H=0$, with $\Phi_r^{1,2}$ given by the simplified form

$$\Phi_r^{1,2}_{H=0} = -\frac{2\sigma^2\xi^2}{(\varepsilon+1)^3} \times \int \int_{0<k,Q<k_e} \frac{kQ^2e^{-k\xi}}{(1+aQ^2+a\xi^2k^2)} \times T_{1,2}(k,Q)dQdk,$$

with $T_{1,2}$ given by $T_1(k,Q)=(1-B^2)^{-1/2}(e(e-1)+[4eB^{-1}+(e-1)B^{-2}]/(1-B^{-2})^{1/2}-1)$, and $T_2(k,Q) = (e-1)[1-(1-B^2)^{-1/2}]B^{-1}+B^{-2}-(1-B^{-2})^{-1/2}$.

Finally, we will comment on the roughness effects on the binding efficiency of the electrostatic-image potential. If we consider the case of electrons ($q<0$), we have $q\Phi_f^2<0$ and $q\Phi_r^2>0$. As a result, interface roughness makes the image potential outside the dielectric interface more attractive to a degree that depends mainly on the long-wavelength roughness features and the distance of the image charge to the point where the potential is determined relative to $\xi$. However, inside the medium the electrostatic potential becomes less attractive to a degree that also significantly depends on the short-wavelength roughness characteristics.

**V. CONCLUSIONS**

We combined knowledge of basic electrostatic theory for the case of rough boundaries with that of analytic height–height correlation models for self-affine fractals in order to investigate quantitatively the effect of the roughness parameters $H$, $\sigma$, and $\xi$ on the electrostatic-image potential of a point charge situated in the vicinity of a dielectric medium. In general, the roughness contribution could be significant ($>10\%$) depending on the distance of the image charge to the point where the potential is determined relative to the roughness correlation length.

Our results show that the dominant effect on the electrostatic potential outside the medium arise from the long-wavelength roughness features ($\sigma, \xi$) and the relative distance $s=(|z|+|z'|)/\xi$, whereas the roughness exponent $H$ has a rather weak contribution. However, inside the dielectric medium the effect of $H$ on the electrostatic potential could be of comparable strength to that of the correlation length $\xi$ and the relative distance $s$, indicating that short-wavelength roughness features could play a significant role on the electrical properties of matter.

Surface/interface roughness, therefore, has to be considered seriously for precise modeling of electrical properties of
matter whenever surface/interface boundaries are involved. Moreover, it would be interesting in the future to examine self-affine roughness effects in physically important systems such as the binding of electrons near the surface of liquid He, the shifting of the electronic levels in the inversion layer of a semiconductor–oxide interfaces, and the motion of charged particles above solid surface.2–5

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APPENDIX: PERTURBATIVE EXPANSIONS

The determination of $A(k)$ and $B(k)$ in Eq. (3) is performed in a perturbative manner up to second order: $A(k) = A_0(k) + A_1(k) + A_2(k)$ and $B(k) = B_0(k) + B_1(k) + B_2(k)$. These expansions are substituted into Eq. (3) to yield $\Phi$ for weak roughness, $|\nabla h|<1$, which leads to $\tilde{\Phi} \approx (\tilde{h}(k_0) + \tilde{h}(k_1) + \tilde{h}(k_2))$. Moreover, we consider the Fourier transform definition $\tilde{h}(r) = (2\pi)^{-2} \int h(k) e^{ik\cdot r} d^2k$. By the subsequent substitution of the perturbative expression of $\Phi$ into the boundary conditions given by Eq. (2), we obtain up to second order (by considering the expansion $e^{\pm kh(r)} \approx 1 \pm kh(r) + (1/2)k^2h(r)^2$ with $kh<1$) $1$

$$[A_0(k), B_0(k)] = \frac{2\pi q}{(1+\epsilon)k} e^{-ik\cdot r' - k\cdot z'} (1-\epsilon, 2),$$

$$[A_1(k), B_1(k)] = -\frac{4\pi q(\epsilon - 1)}{(1+\epsilon)^2} \int e^{-iQ\cdot r' - Q\cdot z'} h(k - Q)$$

$$\times (e^\epsilon + e^{\epsilon\cdot k\cdot \hat{k}} - 1 + e^{\epsilon\cdot \hat{k}\cdot \hat{k}}) \frac{d^2Q}{(2\pi)^2},$$

$$[A_2(k), B_2(k)] = -\frac{4\pi q(\epsilon - 1)}{(1+\epsilon)^3} \int \frac{d^2Q'}{(2\pi)^2}$$

$$\times \int e^{-iQ'\cdot r' - Q'\cdot z'} h(k - Q) - Q'h(Q' - Q)(D_1, D_2),$$

with $\{\hat{Q}, \hat{Q}', \hat{k}\}$ unit vectors, $D_1 = e(\epsilon - 1) + 2e\hat{Q}'(\hat{k} + \hat{Q}')$ and $D_2 = -e(\epsilon - 1) - 2\hat{Q}' \cdot \hat{k} + 2e\hat{Q}' \cdot (\hat{Q}' \cdot \hat{k})(\epsilon - 1)$. Finally, we would like to note that the expansion of $e^{\pm kh(r)}$ up to second order implies that the inequality $k\sigma<1$ must be satisfied as an order of magnitude. Ensemble average over roughness realizations assuming the roughness to be statistically stationary up to second order $\langle h(k)h(k') \rangle = (2\pi)^2 \delta(k + k') \langle |h(k)|^2 \rangle$, yields $\langle A_0(k) \rangle = A_0(k)$, $\langle B_0(k) \rangle = B_0(k)$, $\langle A_1(k) \rangle = \langle B_1(k) \rangle = 0$ since $\langle h(k) \rangle = 0$, and

$$\langle [A_2(k), B_2(k)] \rangle = -\frac{q(\epsilon - 1)e^{-ik\cdot r' - k\cdot z'}}{\pi(1+\epsilon)^3} \int_{0<\theta<\pi} dQ$$

$$\times \int_{0<\theta<2\pi} d\theta Q^2 \langle |h(k - Q)|^2 \rangle D_{1,2}(\theta),$$

$$D_1(\theta) = e(\epsilon - 1) + 4e \cos \theta - (\epsilon - 1) \cos^2 \theta,$$

$$D_2(\theta) = (\epsilon - 1)(2 \cos \theta - \cos^2 \theta - 1),$$

and $\hat{Q} \cdot \hat{k} = \cos \theta$.


6 P. Meakin, Phys. Rep. 235, 1991 (1993); J. Krim and G. Palasantzas, Int. J. Mod. Phys. B 9, 599 (1995) (schematics similar to Fig. 1 in this work that show the effect of $H$ can also be found in Fig. 1 of this reference); G. Palasantzas and J. Krim, Phys. Rev. Lett. 73, 3564 (1994).


