Impact of interfacial roughness on tunneling conductance and extracted barrier parameters

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The net tunneling conductance of metal-insulator-metal tunnel junctions is studied using a distribution of barrier thicknesses consistent with interfacial roughness typical of state-of-the-art tunnel junctions. Moderate amounts of roughness cause the conductance to resemble that of much thinner and taller barriers. Fitting numerically generated conductance data that include roughness with models that assume a single-thickness barrier leads to erroneous results for both the barrier height and width. Rules of thumb are given that connect the roughness to the real space mean thickness and the thickness inferred from fitting the net conductance with traditional tunneling models. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2431443]

Electron tunneling in metal-insulator-metal (MIM) junctions is one of the most fundamental problems in physics that also has broad applications.[1] Tunneling characteristics are generally fit to WKB-based models, such as those of Brinkman-Dynes-Rowell[2] (BDR) or Simmons,[3] using the thickness (s) and interfacial barrier heights (ϕ_1 and ϕ_2) as adjustable parameters. These two models have nearly 1500 combined citations to date and have been employed in normal metal, superconducting, semiconducting, molecular, and magnetic tunnel junctions (MTJs) composed of literally hundreds of different electrode and barrier material combinations. These models assume a single-thickness barrier. However, interfacial roughness cannot be avoided during the growth of multilayered heterostructures, even in epitaxial systems.[4] Simple but realistic models of film deposition predict pinholes that can dramatically change conduction properties; pinholes mimic the exponential decay in current with thickness,[5] which led to a modification of the tunneling criteria for MTJs.[6] Without pinholes, roughness can affect the transport properties of MIM tunnel junctions because of the exponential dependence of the transmission probability on thickness. For example, Da Costa *et al.* used local probes to demonstrate that barrier inhomogeneity results in large distributions of the current in half-formed junctions,[7] while Buchanan *et al.* showed that barrier thicknesses determined from tunneling measurements were systematically lower than the thicknesses measured by x-ray reflectivity.[8] Recently, the existence of parabolic tunneling conductance to anomalously high biases was reported in magnetic[9] and superconducting[10] tunnel junctions. The former showed that this effect originates from interfacial roughness and that the prepared barrier thickness could be recovered from transport measurements only if roughness was explicitly considered.

This letter reports that interfacial roughness not only affects the bias dependence of the tunneling conductance (G) but also leads to erroneous barrier parameters when analyzed with single-thickness models. The calculated net conductance including roughness (G_{net}) at low biases strongly resembles the single-thickness conductance of a barrier that is thinner than the mean of the distribution. We quantify the resulting barrier parameter errors caused by this similarity and offer rules of thumb to estimate the roughness based on the thickness inferred from conductance measurements and the real space mean barrier thickness. Statistical arguments reveal that the uniqueness of fit parameters is a strong function of the bias range used for fitting normalized conductance data.

The tunneling current density for MIM junctions was numerically calculated using the BDR model:[2]

$$j = \frac{2e}{h}\int\int \exp\left(-\frac{2}{\hbar}\int_0^s \sqrt{2m\phi(x,V,E)}dx\right) \times[f(E(k)) - f(E(k) - |e|V)]dEdk. \quad (1)$$

Here, s is a single barrier thickness, $\phi(x,V,E)$ is the position-dependent barrier height for bias V for an electron with incident energy E, e is the elementary charge, m is the free electron mass, k are the wave vectors parallel to the junction interface, and f is the Fermi function. Unlike its quadratic expansion [Eq. (7) in Ref. 2], the validity of Eq. (1) is independent of the barrier height. To simulate the effect of roughness, we calculated the current density via Eq. (1) for a distribution of barrier thicknesses s_n by weighting each individual current density $j(s_n)$ with a thickness-dependent coefficient and summing these as parallel conduction channels. The net conductance G_{net} was obtained from the net current density $j_{\mathrm{net}}=\Sigma_n \alpha(s_n) j(s_n,\phi,V)$, with the nth channel weighted by a coefficient $\alpha(s_n)$ that is obtained from a Gaussian distribution of thicknesses centered at mean thick-

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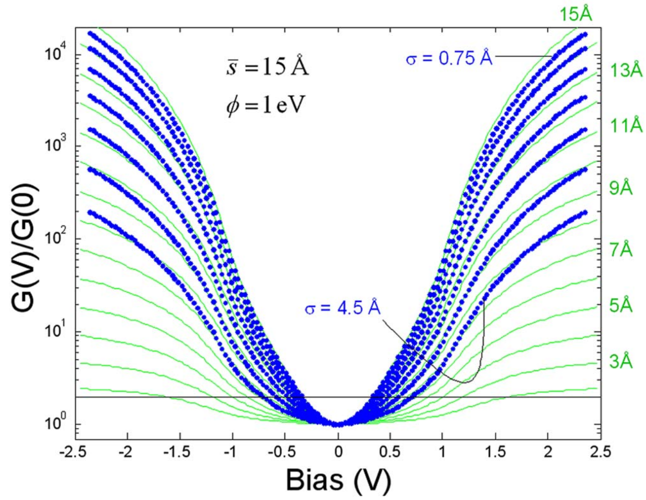

FIG. 1. (Color online) Bias dependence of normalized tunneling conductance, calculated for $\bar{s}=15$ Å, $\phi=1.0$ eV, and σ of 5%–20% of $\bar{s}$ in steps of 2.5% (blue points), and single-thickness ($\sigma \equiv 0$) conductance for 2–15 Å in 1 Å steps (solid green lines).

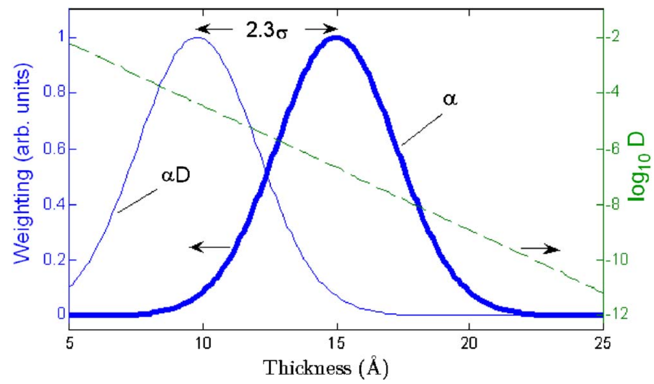

FIG. 2. (Color online) Gaussian weighting coefficients $\alpha(s_n)$ used to simulate roughness (thick line), and tunneling probability $D(s)$ (dashed line) as functions of barrier thickness with $\phi=1$ eV and $s_n=15$ Å$\pm 15\%$. The contribution of each thickness to $G_{\rm net}$ is given by $\alpha \cdot D$ (thin solid line, normalized). The thickness inferred from conductance measurements is the mean of the thin curve, which differs from $\bar{s}=15$ Å by 2.3σ.

ness $\bar{s}$ with the standard deviation σ defining the roughness. The distribution $s_n=\bar{s}\pm\sigma$ represents variations of the barrier thickness over the entire junction area and at both interfaces. One can interpret the weighting coefficients as the relative area of each conduction channel.[11] A thickness step size $(\Delta s = s_i - s_{i-1})$ of 0.5 Å was used because the results were independent of Δs less than this value. This formalism is general for asymmetric barriers; however, we assume a symmetric barrier at zero bias for computational ease. We do not consider ϕ distributions for simplicity, though recent scanning tunneling microscopy work on partially formed MgO-based junctions showed that barrier height distributions do exist ($\phi \sim 0.75 \pm 0.1$ eV in that work for a 15 Å barrier).[12]

Figure 1 shows the bias dependence of the normalized tunneling conductance using the BDR model calculated for a barrier with $\phi=1$ eV, $\bar{s}=15$ Å, and roughnesses of up to $\sigma = \bar{s}\times 20\%$. Roughness causes the conductance to "flatten" and "open up," as if the barrier were thinner. To illustrate this, conductance curves for ideal single-thickness barriers (i.e., $\sigma \equiv 0$) are plotted for comparison (thin lines). For all ϕ and s, the net conductance with $\sigma > 0$ is bounded above by that with $\sigma \equiv 0$, if $eV < \phi$. This is expected because thinner regions dominate the net current due to the exponential dependence of the tunneling probability on thickness.

The weighting coefficients $\alpha(s)$, the tunneling probability $D(s,\phi)$, and their product are shown as functions of s for $\phi=1$ eV, $\bar{s}=15$ Å, and $\sigma=\bar{s}\times 15\%$ in Fig. 2. $D(s,\phi)$ represents the exponential term in Eq. (1), and $\alpha \cdot D$ is thus the integrand of that equation (neglecting the Fermi term). The mean of the $\alpha \cdot D$ distribution is thus the thickness that contributes the most to the net tunneling current density. The thin curve in Fig. 2 shows that an experimentally reasonable roughness of 15% shifts the mean of the $\alpha \cdot D$ distribution to $\bar{s}-2.3\sigma$. This implies that regions of the sample thinner than the real space mean barrier thickness (i.e., "hot spots") will heavily influence the net conductance. As discussed below, this may result in significant errors (35% in this example) when assuming a unique barrier thickness in the presence of a thickness distribution.

The net conductance calculated including roughness closely resembles that for a single-thickness barrier when $eV < \phi$. Thus, modeling these data under the (faulty) assumption of a unique barrier thickness would produce a statistically good fit, though the resulting thickness would differ from the mean of the real space thickness distribution ($\bar{s}$). Figure 3 illustrates this by showing the best fit parameters as functions of $\bar{s}$ and σ when the net conductance for $\phi=1$ eV is fit with the BDR model ($\sigma \equiv 0$) in a bias range of ± 2 V. From this single-thickness perspective, increasing roughness causes a reduced effective thickness and an increased effective barrier height. This is qualitatively reasonable because the bias dependence of G is reduced with thinner and/or taller barriers. Therefore, fitting data that include roughness with a single-thickness model will yield thinner than expected thicknesses,[8] and taller than expected heights. In fact, an empirical relationship is found between $\bar{s}$, σ, the best fit single thickness (s^*), and ϕ that allows the roughness to be estimated when the other parameters are known. Assuming $\phi=1$ eV, the roughness can be estimated with $\sigma(\sigma+1) = 1000(1-s^*/\bar{s})$, where the units of σ are percent of $\bar{s}$. A similar expression for $\phi=4$ eV, near that of ideal MgO,[13] is $\sigma(3\sigma-2)=1000(1-s^*/\bar{s})$. These rules of thumb are accurate to about 10% for $\sigma < 15\%$, and $\bar{s} \leq 20$ Å, and are specific for the stated heights.

Roughness induces a deviation from single-thickness behavior for biases near and above the barrier height. This is

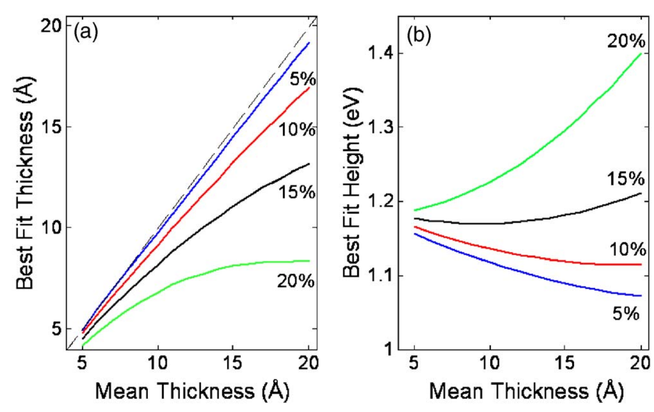

FIG. 3. (Color online) Best fit single thickness (a) and height (b) using the BDR model to fit $G_{\rm net}$ vs V in ± 2 V as a function of $\bar{s}$ with $\phi=1.0$ eV for various σ (in percent of $\bar{s}$).

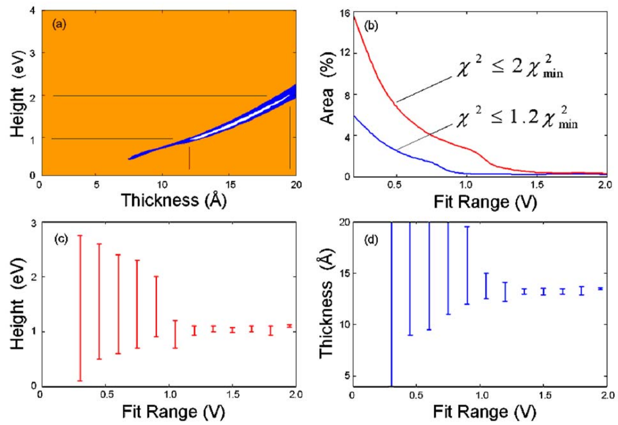

FIG. 4. (Color online) (a) χ^2 parameter space from fitting G_{net} with the full BDR model in a bias range of ±0.9 V: white, blue, and orange filled contours represent $\chi^2/\chi^2_{min} \leqslant 1.2$, $\chi^2/\chi^2_{min} \leqslant 2$, and $\chi^2/\chi^2_{min} > 2$. The solid lines indicate 20% confidence intervals (CI). G_{net} was calculated using $\phi = 1$ eV, and $s = 15$ Å ± 10%. (b) Parameter space area for $\chi^2 \leqslant 1.2\chi^2_{min}$ and $\chi^2 \leqslant 2\chi^2_{min}$ decreases with increasing bias range used for fitting. 20% CI for (c) ϕ, and (d) s as functions of the bias range used for fitting; CI fluctuations are due to using discrete ϕ and s in the calculations.

evidenced by G_{net} crossing single-thickness G curves at high biases in Fig. 1. This implies that the net conductance is not simply dominated by the thinnest channels but rather that the contribution of an individual conduction channel changes with applied bias. The bias dependence of the tunneling probability and the bias independence of the weighting coefficients result in a bias-dependent mean of the $\alpha \cdot D$ distribution that approaches $\bar{s}$ with increasing bias. This causes deviations from single-thickness behavior with increasing bias.

Studying the χ^2 parameter space reveals that uniqueness is a significant problem when the bias range over which the data are fit (V_{fit}) is small compared to ϕ. G is approximately quadratic in this regime, allowing $G/G(V=0)$ to be fit equally well by any member of the family of curves $a = s/\sqrt{\phi}$, where a is a constant. Figure 4(a) shows the χ^2 space when $G/G(V=0)$ of a barrier with $\phi = 1$ eV and $s = 15 \pm 1.5$ Å is fit using the BDR model in a bias range of ±0.9 V. The filled contours show ranges of χ^2 relative to the best value (χ^2_{min}), which was found for $\phi = 1.15$ eV and $s^* = 14.0$ Å. The white, blue, and orange areas indicate χ^2/χ^2_{min} less than 1.2, less than 2, and greater than 2. Figure 4(b) shows that the area of these regions (relative to the ϕ-s parameter space with $\phi \in [0,4]$ eV, and $s \in [0,20]$ Å) decreases significantly when V_{fit} approaches and exceeds the barrier height. This is supported by the 20% confidence intervals for ϕ and s converging for $V_{fit} > \phi$ [Figs. 4(c) and 4(d)]. Note the bias range used for Fig. 3 was ±2 V, which indicates that those best fit parameters were unique. This uniqueness problem is important to note because conductance data are often presented in "arbitrary units." Since fitting details are usually neglected, it is not unreasonable to suppose that fittings are performed to $G/G(V=0)$ and that the resulting barrier parameters may not be unique. Fitting raw data resolves the uniqueness problem in all bias ranges, but as noted above, the best fit parameters are dramatically affected by roughness.

In summary, a distribution of barrier thicknesses was employed to simulate the effect of experimental roughness on the net tunneling conductance for metal-insulator-metal junctions with constant barrier heights. A moderate amount of roughness was shown to significantly alter the net tunneling conductance. For applied biases less than the barrier height, the net conductance resembles that of a barrier whose effective thickness is nearly two-and-a-half standard deviations below the mean thickness for a 15% roughness parameter. Rules of thumb were given to connect the barrier roughness to the real space mean thickness and the thicknesses inferred from conductance measurements. For conductance calculations that include roughness, fits to models that assume a single-thickness barrier lead to errors in both the barrier thickness and height. The uniqueness of fits to normalized conductance data was shown to be a significant problem when the bias range used for fitting was small compared to the barrier height, but not when the bias range exceeds the height.

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