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Subthreshold characteristics of ballistic electron emission spectra

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We report upon a comprehensive investigation of the subthreshold characteristics of the ballistic electron emission microscopy (BEEM) current in ballistic electron emission spectroscopy. Starting from the Bell-Kaiser model, we derive an analytical equation to describe the subthreshold behavior of the BEEM current. It is found that the BEEM current in this region should exhibit a subthreshold swing of \( \sim 60 \text{ mV/decade} \) at room temperature, which we experimentally verified. This finding provides a rule of thumb for the detectability of the subthreshold behavior in a spectrum. For spectra where the subthreshold behavior is discernible above the signal noise, it is demonstrated that significant deviations in the near-threshold region can occur when fitting with a simple quadratic model that ignores the subthreshold behavior. To take the subthreshold behavior into account, a simple analytical model is proposed. This model not only fits significantly better in the near-threshold region than the square model, but also gives a barrier height closer to the one extracted from the Bell-Kaiser model. More significantly, this model provides a quick method to estimate the subthreshold BEEM current amplitude based on the BEEM current above the barrier height.

I. INTRODUCTION

Ballistic electron emission spectroscopy (BEES) is a powerful technique for determining the Schottky barrier height of metal/semiconductor devices with nanometer lateral resolution. In a basic metal/semiconductor configuration, a negatively biased scanning tunneling microscope (STM) tip injects electrons into a grounded thin metal film on a semiconductor substrate. After transport in the thin metal film, some electrons can reach the metal/semiconductor interface without losing significant energies. Electrons with energy above the interface barrier height have a finite probability to transmit across the interface and contribute to the BEEM current. The Bell-Kaiser model, based on the planar tunneling theory in STM, has been successful in modeling the near threshold behavior of the BEEM spectra and extracting the barrier height to a large extent. A simplified power law model (power, \( n = 2 \)) based on the Bell-Kaiser model, has been widely used to fit the spectra, largely due to its simplicity. However, the \( n = 2 \) model is usually based on the assumption of temperature, \( T = 0 \text{ K} \). At non-zero temperatures, there are still electrons above the Fermi energy of the STM tip, as governed by the Fermi-Dirac distribution. When the tip bias is lower than the interface barrier height, these electrons still have a finite probability to reach the metal/semiconductor interface and are collected as the BEEM current. Therefore, it is expected that there will be a non-zero BEEM current when the tip bias is a few \( kT \) (\( k \) is Boltzmann’s constant and \( T \) is the temperature) below the barrier height. Deviations in the fitting of the near (both below and above) threshold region are thus expected when using the \( n = 2 \) model to fit the spectra acquired at a non-zero temperature. Despite these deviations, so far there has been little detailed quantitative study on this subthreshold behavior.

This work has two objectives: First, we will present a quantitative study on the subthreshold characteristics of the BEEM spectra, based on a simplified analytical model derived from the Bell-Kaiser formula. It will be analytically and experimentally shown that the BEEM current in this region decreases at a subthreshold swing (SS) of \( \sim 60 \text{ mV/decade} \), i.e., the BEEM current decreases one order of magnitude when the tip bias decreases by \( \sim 60 \text{ mV} \). It will also be shown that significant deviations could exist when the experimental BEEM spectra are fitted using the simplified \( n = 2 \) model. The second objective of this work is to introduce a simple, but more accurate analytical model for the BEEM spectra fitting. As an extension of the \( n = 2 \) model, the proposed model includes the temperature dependence and takes into account the subthreshold characteristics. We will show that this model significantly improves the fitting accuracy in the near-threshold region and the extracted barrier heights are very similar to those extracted from the full Bell-Kaiser model. We will also show that this model provides a method to quickly estimate the BEEM current in the subthreshold region based on the BEEM current at 10 \( kT \) above the extracted barrier.

II. SUBTHRESHOLD CHARACTERISTICS

The Bell-Kaiser model for the BEEM spectra of a metal/n-type semiconductor device at a constant tunneling gap based on the planar tunneling theory can be written as:

\[
I = \frac{e^2}{2\pi^2\hbar^2} \frac{1}{V^2} \left[ \frac{1}{n^{\alpha}} - \frac{1}{(n+1)^{\alpha}} \right] \exp\left(-\frac{eV}{kT} - \frac{n}{n+1} \right)
\]

where \( n \) is the effective density of states, \( V \) is the voltage, \( V_0 \) is the barrier height, and \( \alpha \) is the barrier height exponent. The subthreshold characteristics are characterized by the subthreshold swing (SS) defined as the voltage swing required for the current to decrease by two orders of magnitude. In the Bell-Kaiser model, the subthreshold swing is given by

\[
SS = \frac{e}{kT} \ln(10) \left( \frac{n+1}{n} \right)^{\alpha}
\]

This expression is valid for arbitrary values of \( n \) and \( \alpha \). However, in practice, \( n \) is often assumed to be 2, and \( \alpha \) is typically close to 2. The subthreshold swing then simplifies to

\[
SS = \frac{e}{kT} \ln(10) \left( \frac{3}{2} \right)^{\alpha}
\]

For a metal/metal Schottky barrier, the subthreshold swing is simply

\[
SS = \frac{e}{kT} \ln(10) \left( \frac{3}{2} \right)^{\alpha}
\]

In the Bell-Kaiser model, the subthreshold swing is constant and independent of the barrier height.

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\]

In the Bell-Kaiser model, the subthreshold swing is constant and independent of the barrier height.
where \( I_{\text{BEEM}} \) is the BEEM current, \( R \) is an attenuation factor accounting for the electron transport through the metal and the metal/semiconductor interface, \( C \) is a constant, \( f(E) \) is the Fermi–Dirac distribution function, \( T(E_{\text{cm}}) = e^{-2\sigma}/[1+(1/4)e^{-2\sigma}] \) is the tunneling probability through the vacuum gap based on the Wentzel–Kramers–Brillouin (WKB) approximation,\(^6\) with

\[
\sigma = -\frac{2}{3}\frac{d}{eV}\sqrt{\frac{\hbar^2}{2m}} \left[ (E_F + \varphi - eV - E_{\text{cm}})^{3/2} - (E_F + \varphi - E_{\text{cm}})^{3/2} \right].
\]

Here, \( d \) is the vacuum gap width, \( \hbar \) is the reduced Plank’s constant, \( \varphi \) is the average workfunction of the tip and the metal base, \( E_{\text{cm}} \) and \( E_{\text{m}} \) are the perpendicular and transverse energy components of the electrons in the metal base, respectively, \( E_{\text{cm}}^\text{min} = E_F - eV + \Phi_{\text{BH}} \) and \( E_{\text{cm}}^\text{max} = m/m - m_{\text{t}} \) (\( E_{\text{cm}} + eV - E_F - \Phi_{\text{BH}} \)), \( E_F \) is the Fermi energy of the tip, \( e = +1.6 \times 10^{-19} \) C is the elemental charge, \( V \) is the absolute value of the tip bias, \( \Phi_{\text{BH}} \) is the interface barrier height, \( m_{\text{t}} \) is the transverse electron effective mass parallel to the interface in the semiconductor, and \( m \) is the free electron mass.

To compensate for the change in the tunneling gap during the acquisition of the BEEM spectra under constant tunneling current condition, Bell and Kaiser\(^2\) proposed the following formula, which basically modified Eq. (1) by dividing it by the tunneling current at each tip bias at the same tunneling gap,

\[
I_{\text{BEEM}} = \frac{R}{E_{\text{cm}}^\text{max}} \int_{E_{\text{cm}}^\text{min}}^{E_{\text{cm}}^\text{max}} \int_{0}^{\infty} T(E_{\text{cm}}) \left[ \int_{0}^{E_{\text{cm}}^\text{max}} [f(E) - f(E + eV)] dE_{\text{cm}} \right] dE_{\text{cm}},
\]

(2)

where \( R \) is a constant to be determined from the fitting. Note also that the tunneling current setpoint, \( I_0 \), has been dropped here for the convenience of discussion.

To derive an analytical model for the subthreshold characteristics of the BEEM spectra, we first consider Eq. (1): for \( eV \gg kT \), \( f(E + eV) \) can be neglected compared to \( f(E) \), thus the inner integral of Eq. (1) can be written as,

\[
\int_{0}^{E_{\text{cm}}^\text{max}} [f(E) - f(E + eV)] dE_{\text{cm}} \approx \int_{0}^{E_{\text{cm}}^\text{max}} f(E) dE_{\text{cm}}.
\]


Note that we are considering \( eV \leq \Phi_{\text{BH}} \), so \( E_{\text{cm}}^\text{min} = E_F - eV + \Phi_{\text{BH}} \geq E_F \), i.e., \( E_{\text{cm}} - E_F \geq 0 \). In addition, the inner integral we are considering will be later integrated from \( E_{\text{cm}}^\text{min} \) to infinity (in practice, to a value larger than a few \( kT \) above \( E_F \), e.g., 1) with respect to \( E_{\text{cm}} \). The minimum value for \( E_{\text{cm}}^\text{max} \) is zero, however, for the majority of the \( E_{\text{cm}} \) values in the interval of \( [E_{\text{cm}}^\text{min}, E_{\text{cm}} + 1] \), \( E_{\text{cm}}^\text{max} \) is much larger than \( kT \). For these \( E_{\text{cm}} \) values, \( \exp(-E_{\text{cm}}^\text{max} + E_{\text{cm}} - E_F/kT) \gg \exp(-E_{\text{cm}}^\text{max} + E_{\text{cm}} - E_F/kT) \). Thus, Eq. (3) can be written as,

\[
\int_{0}^{E_{\text{cm}}^\text{max}} f(E) dE_{\text{cm}} \approx kT \ln \left[ \frac{E_{\text{cm}} - E_F}{kT} + 1 \right].
\]

(4)

With the preceding approximation, Eq. (1) can be written as,

\[
I_{\text{BEEM}} = RCKT \int_{E_{\text{cm}}^\text{min}}^{E_{\text{cm}}^\text{max}} T(E_{\text{cm}}) \exp \left[ \frac{E_{\text{cm}} - E_F}{kT} \right] dE_{\text{cm}}.
\]

(6)

Since \( T(E_{\text{cm}}) \) changes much more slowly compared to the exponential term (this can be easily verified by plotting the \( T(E_{\text{cm}}) \approx E_{\text{cm}} \) curve), it can be approximated to be a constant. Equation (6) can be then written as,

\[
I_{\text{BEEM}} \approx C \int_{E_{\text{cm}}^\text{min}}^{E_{\text{cm}}^\text{max}} \exp \left[ \frac{E_{\text{cm}} - E_F}{kT} \right] dE_{\text{cm}}.
\]

(7)

where \( C \) is a constant. This suggests that the BEEM current in the subthreshold region increases exponentially with the tip bias with a subthreshold swing of

\[
\text{SS} = \text{dlog}_{10} I_{\text{c}}/\text{dV}^{-1} = \ln 10 (kT/e) \approx 60 \text{ mV/decade} \text{ at room temperature}.
\]

In other words, the BEEM current in the subthreshold region decreases one order of magnitude when the tip bias (the absolute value) decreases by \( \approx 60 \text{ mV} \).

Now we consider the subthreshold characteristics of the BEEM spectra described by Eq. (2), i.e., the Bell–Kaiser model for constant tunneling current. The tunneling current at a constant tunneling gap usually changes only about one order of magnitude or less under normal experimental spectrum conditions. Thus, the normalization by the tunneling current does not significantly change the overall exponentially increasing behavior of the BEEM current in the subthreshold region, except that it will slightly change the subthreshold swing (this will also be further verified by the simulation results later).

In order to further verify that the approximations made previously are indeed reasonable, we will consider the simulated BEEM spectra based on Eqs. (1) and (2).

Figure 1(a) is a simulated BEEM spectrum for an Au/n-Si system plotted in both linear and logarithmic-linear scale based on the constant gap BEES described by Eq. (1). Here,
Figure 1(b) is another simulated BEEM spectrum for an Au/n-Si system plotted in both the linear and logarithmic-linear scale based on the constant current BEES described by Eq. (2). All of the parameters used were the same as those used in Fig. 1(a). The black solid line in the range of 0.356–0.856 V in the logarithmic-linear scale curve is a linear fit of $\log_{10}(I_{\text{BEEM}})$ vs. $V$. The fitting gave a subthreshold swing of 64.4 mV/decade. If the fitting was limited to the range of 0.04 V below the barrier height, i.e., 0.816–0.856 V, the extracted subthreshold swing would be 69.8 mV/decade. This verifies that the normalization by the tunneling current in Eq. (2) does not change the overall exponential behavior of the BEEM spectra in the subthreshold region; however, it slightly changes the subthreshold swing.

### III. EXPERIMENTAL VERIFICATION

#### A. Experimental details

In order to test the preceding simulation results, we carried out an experiment on an Au/n-Si(111) sample. The n-Si(111) substrate was first etched with a buffered hydrofluoric acid and then loaded into an ultrahigh vacuum (UHV) preparation chamber with a base pressure of $3 \times 10^{-10}$ mbar. A gold film 5 nm thick and 0.5 mm in diameter was then deposited by thermal evaporation onto the silicon substrate without any other prior treatment. After the deposition, the sample was transferred in situ into the RHK UHV STM chamber for the BEEM measurements. A chemically etched W tip that was cleaned by electron-bombardment in UHV was used for the measurements. All of the BEEM results presented here were acquired at room temperature with a negative tip bias.

#### B. Experimental verification of the subthreshold characteristics

In order to verify the subthreshold characteristics described by both Eqs. (1) and (2), we acquired BEES at both constant tunneling gap and constant tunneling current conditions.

Figure 2(a) is the zoomed-in view of the subthreshold region of a typical spectrum (an average of a few spectra at the same location) taken at a constant gap condition (i.e., the feedback loop was off). The setpoint was at the tip bias, $V_{\text{tip}} = -0.1$ V, and the tunneling current, $I_t = 1$ nA. The acquisition of the BEEM spectra at the constant gap at room temperature is much more difficult than acquiring it at the constant current condition, largely due to the drift issue. The spectra presented here were carefully checked to ensure that the forward and backward sweeps were nearly identical, i.e., the drift is minimized. The inset is the full spectrum with the fit. The fit (black solid line) was carried out using Eq. (1) with the $R$ factor and the barrier height as two adjusting parameters and all other parameters are the same as those used in the simulation in Fig. 1. The fitting range was limited to 0.2 eV with $\phi$ set self-consistently above every barrier height being evaluated. The extracted barrier height was 0.856 eV and the corresponding tip bias is indicated by the vertical blue dotted line. The vertical green line corresponds to the value of 60 mV below the extracted barrier height. It can be seen that

![Figure 1](image-url)
the fitting with the constant gap Bell-Kaiser model was reasonably good in both the region above the threshold and in the subthreshold region. The enlarged view of the subthreshold region also shows that the BEEM current in the subthreshold region exponentially decreases at a rate of about 60–70 mV/decade.

To have a more direct and quantitative test of the simulation results, a linear fit of $\log_{10}(I_{\text{BEEM}})$ vs. $V$ was performed for the experimental data in the range of 0.816–0.856 V (40 mV below the extracted barrier height), as shown in Fig. 2(b). The extracted subthreshold swing was 68.3 mV/decade, which is very close to the one extracted in Fig. 1(a) in the same fitting range.

Figure 3(a) is a close-up view of the subthreshold region of a typical spectrum (an average of a few spectra) taken at a tunneling current condition of $I_t = 5$ nA, while the inset is the full spectrum. The fitting (black solid line) was carried out in the same way as the spectrum in Fig. 2(a), except that this fitting used Eq. (2), i.e., the Bell-Kaiser model for the constant tunneling current. The extracted barrier height was 0.834 eV and the corresponding tip bias is indicated by the vertical magenta dotted line. The vertical blue line corresponds to the value of 60 mV below the extracted barrier height. It can be seen that the fitting with the Bell-Kaiser model works reasonably well both in the region above the threshold and in the subthreshold region, as pointed out by other researchers. The enlarged view of the subthreshold region also shows that the BEEM current in the subthreshold region exponentially decreases at a rate of about 60–70 mV/decade.

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A linear fit of $\log_{10}(I_{\text{BEEM}})$ vs. $V$ to the experimental data in the range of 0.795–0.835 V (40 mV below the extracted barrier height), shown in Fig. 3(b), gave a subthreshold swing of 72.0 mV/decade. This is slightly larger than the one extracted from the constant gap BEES in Fig. 2(b). This is expected, as discussed in Sec. II. The extracted subthreshold swing depends weakly on the fitting range and varies slightly between 60–75 mV/decade from spectrum to spectrum.

One important application of the subthreshold Eq. (7) is to estimate the actual tip temperature. For the experiment where the sample is being directly cooled down, but the tip is not, one can estimate the actual tip temperature by fitting the subthreshold region of the BEEM spectra.
IV. A MODEL THAT INCLUDES SUBTHRESHOLD CHARACTERISTICS

A. Comparison on the goodness-of-fit for the subthreshold region

Before we proceed to propose a new model, we will first demonstrate that the square (n = 2) model fits very poorly in the near-threshold region, since it does not consider the subthreshold characteristics.

Figure 4(a) is a close-up view of the same BEEM spectrum as Fig. 2(a) (red circles, the average of a few spectra) acquired at the constant gap condition, with the full spectrum in the inset. The black and blue solid lines are the respective fittings with the n = 2 model and the Bell-Kaiser model at the constant gap (Eq. (1)), and the fitting range was both limited to 0.2 eV self-consistently above every barrier height being evaluated. The barrier heights extracted from the two fittings are 0.822 and 0.856 eV, respectively. The barrier height from the n = 2 model is about 0.03–0.04 eV less than that from the Bell-Kaiser model. The close-up view shows that the Bell-Kaiser model fitted reasonably well in the near threshold region, while significant deviations from the experimental spectrum in this region can be observed for the n = 2 model. This is further confirmed by the square of residuals at each tip bias shown in Fig. 4(b), where the dotted vertical lines are the respective barrier heights extracted.

B. Proposed model

The n = 2 model is widely used to extract the barrier height from the BEEM spectra. However, in the previous section we have demonstrated that this model does not fit the subthreshold region and gives a barrier usually smaller than the one extracted from the full Bell-Kaiser model. Similar problems also occur for other simple models. In order to take the subthreshold BEEM current into account in the fit, we propose the following simple model:

\[
I_{BEEM} = \begin{cases} 
R(kT)^2 \exp\left(\frac{eV - \Phi_{BH}}{kT}\right), & \text{for } eV < \Phi_{BH} \\
R(kT)^2 \left[1 + \left(\frac{eV - \Phi_{BH}}{kT}\right)^2 \right], & \text{for } eV > \Phi_{BH},
\end{cases}
\]

where R is a constant to be determined from the fitting and \(I_{BEEM}\) is the BEEM current. For \(eV \leq \Phi_{BH}\), this model uses Eq. (7) to describe the subthreshold behavior. For \(eV - \Phi_{BH} \gg kT\), the proposed model approaches the n = 2 model. For \(eV\) that is slightly larger (about a few kT or less) than \(\Phi_{BH}\), we still adopt the subthreshold equation. As an approximation, however, the exponential terms are expanded into a power series and only the low order terms (up to second order) are used. In this way, the proposed model approaches the n = 2 model when \(eV = \Phi_{BH}\). Compared to the n = 2 model, this simple model includes the subthreshold characteristics and is temperature dependent.

The green solid line in Fig. 4(a) is the fit with the proposed model. The inset of Fig. 4(a) shows that this model is almost the same as the n = 2 model in the high bias range. Figure 4(a) also shows that the proposed model significantly improves in the fitting of the near threshold region compared to the n = 2 model. This is even clearer by looking at the square of the residuals in Fig. 4(b). Furthermore, the extracted barrier height from the proposed model is 0.862 eV, which is very close to the value from the Bell-Kaiser model.
In the bias a little bit above the threshold (e.g., above 0.92 V), Fig. 4(b) shows that there are certain deviations, even for the Bell-Kaiser model. However, most of these deviations appeared to be common for all three models. A closer look at the original spectra often indicates that this is due to some random small jumps in the spectra which, therefore, cannot be attributed to the fitting models.

C. Linking the subthreshold BEEM current and the BEEM current above the threshold

From Eq. (8) of the proposed model, we can see that the BEEM current is equal to $I_{\text{BEEM}} = R \left( kT \right)^2$ when $V = \Phi_B / e$. When $eV - \Phi_B = -\ln(10)kT \approx -60$ meV at room temperature, the BEEM current will be about $I_{\text{BEEM}} = \ln(10)kT / 10$, and when $eV - \Phi_B = 10kT \approx 0.26$ eV, the BEEM current will be about $I_{\text{BEEM}} = 60I_{\text{BEEM}}$.

To further verify the preceding prediction, the constant gap BEES from Fig. 2(a) is plotted in Fig. 5(a) again, while Fig. 5(b) is a zoomed-in view of the near threshold region. The three vertical dotted lines correspond to the extracted barrier height, 60 mV below the barrier height, and 0.26 V above the barrier height, respectively. The BEEM current at 0.26 V above the barrier is about 98 pA. From the proposed model, we would expect the BEEM current at the barrier height to be around $98/60 \approx 1.63$ pA, while the zoomed-in spectrum in Fig. 5(b) shows that the actual BEEM current is about 2.1 pA. In the subthreshold region, we would expect the BEEM current to be around $1.63/10 \approx 0.16$ pA, while Fig. 5(b) shows that the actual BEEM current is about 0.3 pA. The actual BEEM currents for both of these predictions are within 50% of error.

Given that the proposed model does not fit the subthreshold region as well as the Bell-Kaiser model does, the prediction with the proposed model will not be so accurate. However, as an analytical model and as an approximation, it provides a reasonably good estimation on the subthreshold BEEM current by looking at the BEEM current at 0.26 eV above the barrier for the spectra acquired at room temperature. By comparing the estimated BEEM current and the noise level in the spectrum, one can easily determine if this subthreshold BEEM current can be observed in the experiment. Note that the value of 10 kT is chosen such that it is not far from the barrier so that the fitting does not deviate much from the experimental data at that bias, and it is also not too close to the barrier so that the BEEM current is reasonably high.

Finally, we can see from Eq. (8) that the ratios between the BEEM currents at the three biases do not depend on the material (either metal or semiconductor) used. However, the three tip biases will shift accordingly if a diode with a different barrier height is used.

D. Application to constant current BEES

The BEEM spectra previously shown were mostly taken at the constant gap. However, in practice, ballistic electron emission spectroscopy is usually performed in the constant current condition due to the difficulty in acquiring the constant gap BEES. In this section, we will compare the fittings of the BEES acquired at constant current condition with the three models.

Figure 6(a) is a zoomed-in view of a typical BEEM spectrum (red circles, an average of a few spectra) acquired at $I_t = 5$ nA, with the full spectrum as the inset. The three solid lines are the fittings with the $n = 2$ model, the proposed model, and the Bell-Kaiser model (Eq. (2)), respectively, and the fitting range was limited to 0.2 eV self-consistently above every barrier height being evaluated. The barrier heights extracted from the three fittings are 0.801, 0.831, and 0.835 eV, respectively. The barrier height from the $n = 2$ model is again about 0.03–0.04 eV less than that from the Bell-Kaiser model. The inset illustrates that the Bell-Kaiser model can predict closer to the experimental data in the higher bias range. This is because it has considered the tunneling gap change during the constant current spectrum. The zoomed-in view shows that the Bell-Kaiser model fits very well in the near-threshold region, while significant deviations from the experimental spectrum in this region can be observed for the $n = 2$ model. The proposed model does not fit as well as the Bell-Kaiser model does; however, it has a significant improvement in the near-threshold region compared to the $n = 2$ model. This is further confirmed by the square of the residual at each tip bias shown in Fig. 6(b), where the dotted vertical lines are the...
extracted barrier heights. The fitting range can be higher than 0.2 eV, however, we note that a zoomed-in view of the near-threshold region often shows that the deviation becomes larger when the fitting range increases.

V. CONCLUSION

A simple analytical equation describing the subthreshold behavior is derived from the Bell-Kaiser model, revealing that the BEEM current exponentially decreases with a rate of ~60 mV/decade at room temperature. This is further supported by the experimental data from an Au/n-Si(111) sample. While the complete Bell-Kaiser model fits the experimental data nicely, great deviations could occur when fitting with the simplified square model. We therefore propose a more accurate, yet still simple, analytical model for the BEEM spectra fitting. We have shown that this model significantly improves the fitting in the near-threshold region and gives a barrier height value close to the one extracted from the complete Bell-Kaiser model. More importantly, it provides a quick method to estimate the subthreshold BEEM current based on the BEEM current above the barrier: the BEEM current at the barrier height is about 1/60 times of that at 10 kT above the barrier, while the BEEM current at ln(10)kT below the barrier is about 1/10 times that at the barrier height.

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FIG. 6. (Color online) (a) A zoomed-in view of the near threshold region of a representative BEEM spectrum (circles, average of a few spectra) taken at I_t = 5 nA from a 5 nm Au/n-Si(111) sample. The three solid lines (from lower to upper in the near threshold region) are the fittings with n = 2, the proposed model, and the Bell-Kaiser model (Eq. (2)), respectively, and the fitting range was all was limited to 0.2 eV self-consistently above every barrier height being evaluated. The barrier heights extracted from these fittings are 0.801, 0.831, and 0.835 eV, respectively. They are also indicated by the respective vertical dotted lines. The inset is the full spectrum. (b) The square of the residual at each tip bias for the fitting in Fig. 6(a). The two upper curves are shifted up by 0.1 and 0.2 pA^2, respectively, for clarity.

4Here, threshold is defined as the voltage corresponding to the extracted barrier height value.
5C. Tivarus, Ph. D. thesis (The Ohio State University, Columbus, 2005).
8The extracted barrier heights from the Bell-Kaiser fitting are rather insensitive to the choice of the average workfunction in the range of 3–4.7 eV and the tunneling gap distance of 7–15 Å; this has also been pointed out in Ref. 9.
13In order to improve the fitting in the near threshold region, one can introduce a factor, \( f \approx 1.2 \), to compensate for the approximations made in the model by changing \( (eV - \Phi_{BH})/(kT) \) to \( (eV - \Phi_{BH})/(fRT) \). We find that introducing this factor can improve the fitting in the near threshold region, and the extracted barrier height value does not significantly change (\(~0.01\) eV or less).