# Explanation of the linear correlation between barrier heights and ideality factors of real metal-semiconductor contacts by laterally nonuniform Schottky barriers

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A new and simple-to-use method to obtain homogeneous Schottky barrier heights from effective barrier heights and ideality factors that are determined from current-voltage ($I$-$V$) characteristics of metal-semiconductor contacts is presented. This approach is justified by a theory of metal-semiconductor interfaces with laterally inhomogeneous distributions of barrier heights. Effective barrier heights and ideality factors were determined from $I$-$V$ characteristics of Si and GaN Schottky contacts and a linear reduction of the effective barrier heights with increasing ideality factors was always observed. These findings are explained by numerical simulations of inhomogeneous Schottky contacts which are based on theoretical results by Tung [Phys. Rev. B **45**, 13509 (1992)]. The homogeneous barrier heights of metal-semiconductor contacts are obtained by a linear extrapolation of the effective barrier heights to $n_{if} \cong 1.01$, the value of the ideality factor characteristic for image-force lowering of Schottky barriers only. © *1997 American Vacuum Society.* [S0734-211X(97)07804-9]

## I. INTRODUCTION

Most metal-semiconductor contacts are rectifying.[1] Schottky[2] explained this behavior by depletion layers on the semiconductor side of such interfaces. The band bending in this space-charge region is characterized by its barrier height, which is the energy distance between the Fermi level and the edge of the respective majority-carrier band right at the interface. For moderate doping levels of the semiconductor, tunneling through the barrier may be neglected and thermal emission over the barrier determines the current-voltage ($I$-$V$) characteristics of rectifying metal-semiconductor or Schottky contacts. The image force lowers the barrier height and makes it voltage-dependent. This Schottky effect[3] is accounted for by an ideality factor. Traditionally, rectifying metal-semiconductor contacts are characterized by their barrier heights and ideality factors.

In the past, discussions on the physical mechanisms that determine the barrier heights in Schottky contacts have dominated the field of metal-semiconductor contacts. The metal-induced gap states[4–6] are considered to be the primary mechanism[7] while additional interface dipoles due to interface doping[8] or correlated with specific interface structures,[9–12] as well as fabrication-induced defects,[7] were proposed as secondary mechanisms. Mostly, the interfaces were implicitly assumed to be laterally uniform and the contacts were characterized by their barrier heights and ideality factors. However, Tung *et al.*[13,14] and Rau *et al.*[15] already pointed out that inhomogeneities may play an important role and have to be considered in the evaluation of experimental $I$-$V$ characteristics. The application of standard procedures gives *effective* barrier heights and ideality factors only. Both parameters vary from diode to diode even if they are identically prepared. Only recently, a correlation between effective barrier heights and ideality factors was reported and it was approximated by a linear relationship.[8,11] This finding was attributed to inhomogeneous interfaces and the barrier heights obtained by extrapolation to the ideality factor calculated for image-force lowering only were taken as values characteristic of homogeneous interfaces. It was concluded that these values, rather than mean values obtained from a set of identically prepared contacts of the same kind, should be compared with theoretical results. The purpose of the present article is to analyze this procedure by considering theoretical results obtained by Tung[14] for the current-voltage relationship of nonuniform Schottky contacts. It is worth mentioning that effective barrier heights and ideality factors reported for $Pd_2Si/n$-Si (Ref. 16) and Ni/$n$-GaAs (Ref. 17) Schottky contacts are also linearly correlated. These data were obtained from $I$-$V$ characteristics recorded as function of temperature.

## II. THEORETICAL BACKGROUND

The thermionic-emission theory gives the current across uniform metal-semiconductor interface as[18,19]

$$I = AA_R^{**}T^2 \exp\left(-\frac{\Phi_{B0}^{\mathrm{eff}}}{k_BT}\right)\left[\exp\left(\frac{e_0V_c}{nk_BT}\right)-1\right], \tag{1}$$

where $A$ is the diode area, $A_R^{**}$ is the effective Richardson constant, $T$ is the temperature, $k_B$ is Boltzmann's constant, $e_0$ is the electronic charge, $V_c$ is the voltage drop across the contact, and $\Phi_{B0}^{\mathrm{eff}}$ and $n$ are the effective barrier height and the ideality factor of the contact, respectively. Image-force lowering and generation-recombination currents give ideality factors $n_{if} = 1.01 \div 1.03$ and $n_{rg} = 2$, respectively. These mechanisms are not sufficient to explain the experimental values of $1.01 \leqslant n \leqslant 2$ routinely observed. Moreover, this

[a)]Electronic mail: w.moench@uni-duisburg.de simple thermionic theory fails to account for other anomalies such as, for example, temperature-dependent barrier heights and ideality factors. These problems were overcome by a theoretical approach of Tung's[13,14] who considered nonuniform or "patchy" Schottky contacts.

Initially, inhomogeneous metal-semiconductor contacts were treated as to consist of separate diodes with different barrier heights and areas in parallel. Such models are correct as long as the dimensions of the patches are large compared to the Debye length of the semiconductor. If the size of the patches embedded in much larger areas of higher and uniform barrier height becomes comparable to or even smaller than the Debye length, then saddle-point barriers exist in front of the patches. The barrier height at the saddle point is intermediate between the values of the patch itself and of the surrounding homogeneous contact area. The saddle-point barrier depends on the applied voltage. This results in a "pinch-off" of the patches as the bias increases.

Tung[13] has analyzed the current transport in nonuniform Schottky contacts in great detail. His results explain all the "anomalies" of the barrier height and ideality factor which have been obtained from $I$-$V$ characteristics of metal-semiconductor contacts when they are evaluated by applying Eq. (1). Tung found that, for example, circular inhomogeneities are characterized by the parameter $\gamma=3(R_p^2\Delta_p/4)^{1/3}$, i.e., by the product of the patch area $\pi R_p^2$ and the deviation $\Delta_p$ of their local barrier height from the homogeneous value $\Phi_{B0}$. The subscript 0 refers to zero bias. Tung then assumed patches of area density $\rho_p$ with a Gaussian distribution

$$N(\gamma)=\frac{\rho_p}{\sqrt{2\pi}\sigma}\exp\left(-\frac{\gamma^2}{\sigma^2}\right) \tag{2}$$

of their patch parameters $\gamma$, where $\sigma$ is the standard deviation. The total current through such patchy diodes then results as

$$I_{\text{total}}=AA_R^{**}T^2\exp\left(-\frac{\Phi_{B0}}{k_BT}\right)\left[\exp\left(\frac{e_0V_c}{k_BT}\right)-1\right]\times\left[1+\frac{8\pi\rho_p\sigma^2\eta^{1/3}}{9(V_{b0}-V_c)^{1/3}}\exp\left(\frac{e_0^2\sigma^2(V_{b0}-V_c)^{2/3}}{2(k_BT)^2\eta^{2/3}}\right)\right] \tag{3}$$

with $\eta=\varepsilon_b\varepsilon_0/e_0N_d$ where $\varepsilon_b$ and $N_d$ are the bulk dielectric constant and the dopant density of the semiconductor, respectively, and $V_{b0}$ is the interface band-bending of the uniform barrier outside the patches.

In real Schottky contacts the series resistance $R_s$ of the semiconductor bulk and the measurement setup cannot be omitted.[20] This reduces the applied voltage $V_a$ by $R_sI_{\text{total}}$ and the voltage across the contact itself amounts to $V_c=V_a-R_sI_{\text{total}}$. Equation (3) then becomes an implicit function of the total current and has to be rewritten as

$$I_{\text{total}}=AA_R^{**}T^2\exp\left(-\frac{\Phi_{B0}}{k_BT}\right)\left[\exp\left(\frac{e_0(V_a-R_sI_{\text{total}})}{k_BT}\right)-1\right]\times\left[1+\frac{8\pi\rho_p\sigma^2\eta^{1/3}}{9(V_{b0}-V_a+R_sI_{\text{total}})^{1/3}}\times\exp\left(\frac{e_0^2\sigma^2(V_{b0}-V_a+R_sI_{\text{total}})^{2/3}}{2(k_BT)^2\eta^{2/3}}\right)\right]. \tag{4}$$

Equation (4) completely describes the current through nonuniform Schottky contacts which exhibit circular patches with a Gaussian distribution of the patch parameter $\gamma$. However, Eqs. (3) and (4) do not include the image-force lowering of the barrier heights.

## III. EXPERIMENT

As substrates we used standard $n$-Si(111) wafers (Wacker Chemitronik) and $n$-type $\alpha$-GaN epilayers on sapphire (Cree Research Inc.). Both types of samples were first dipped in hydrofluoric acid which was diluted by a buffered HF solution ($HF:NH_4F:NH_4OH$) with $p$H=9. This procedure leaves the Si samples with hydrophobic Si(111):H-1×1 surfaces. The Si substrates were subsequently transferred into the ultrahigh vacuum (UHV) system and briefly annealed at 850 °C to desorb the hydrogen and to produce clean Si(111)-7×7 surfaces. After the wet chemical treatment the GaN samples were rinsed in de-ionized water, blown dry with $N_2$ gas, and immediately transferred into the UHV system. The GaN substrates were still contaminated by ~1 monolayer of oxygen. It was completely removed during exposure of the GaN samples to a flux of $1\times10^{16}$ Ga atoms/cm$^2$ s at 800 °C for 10 min, which was followed by an annealing in UHV for another 30 min. These surfaces showed sharp 1×1 low-energy electron diffraction (LEED) patterns and their x-ray photon spectroscopy (XPS) spectra revealed no traces of any residual impurities.

Onto the clean Si(111)-7×7 and GaN(0001)-1×1 surfaces, metals were evaporated *in situ* from Knudsen cells through a mask which had circular openings with nominal diameters of 1 mm. The exact diode areas were determined using an optical microscope. The evaporation rates were monitored using a quartz oscillator and were adjusted to 0.05 nm/s. The metal films had a nominal thickness of 150 nm. Ohmic contacts were achieved by rubbing metallic gallium with an Al pencil onto the GaN samples. The Si wafers, on the other hand, exhibited implanted $n^+$ layers on their rear face which acted as Ohmic contacts. The $I$-$V$ characteristics were recorded outside the UHV system and in the dark.

## IV. RESULTS AND DISCUSSION

Figure 1 displays the forward $I$-$V$ characteristic (open circles) of a Sn/Si(111) Schottky contact and a least-squares fit (full line) of Eq. (4) to the experimental data. The fitting parameters were the homogeneous barrier height $\Phi_{B0}$, the series resistance $R_s$, the patch density $\rho_p$, and the standard deviation $\sigma$ of the patch-parameter $\gamma$. The diode temperature was 296 K. The fitting procedure included all experimental

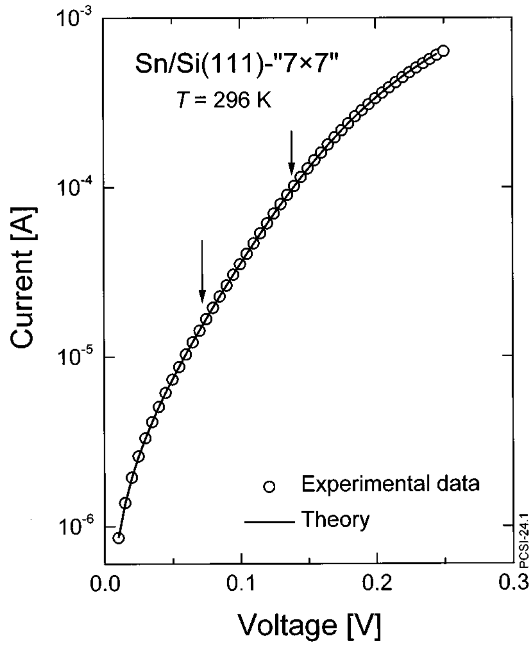


FIG. 1. Current-voltage characteristic of a Sn/Si(111)-"7×7" Schottky diode at room temperature. The full line is a least-squares fit of Eq. (4) to the experimental data with $\Phi_{B0}=0.679$ eV, $\sigma=2.18\times10^{-4}$ $cm^{2/3}$ $V^{1/3}$, $\rho_p=1.79\times10^{7}$ $cm^{-2}$, and $R_s=97$ $\Omega$. The arrows indicate the voltage range from which an effective barrier height $\Phi_{B0}^{eff}=0.62$ eV and an ideality factor $n=1.41$ were calculated using Eq. (1).

data points in the voltage range from 0.01 to 0.25 V. We obtained a homogeneous barrier height $\Phi_{B0}=0.679$ eV, a series resistance $R_s=97$ $\Omega$, a patch density $\rho_p=1.79\times10^{7}$ $cm^{-2}$, and a standard deviation of the patch-parameter $\sigma=2.18\times10^{-4}$ $cm^{2/3}$ $V^{1/3}$. In addition to this fitting procedure we also performed a "standard evaluation" of the $I$-$V$ characteristics using Eq. (1). In the voltage range from 0.075 to 0.14 V, which is indicated by the arrows in Fig. 1, $\ln(I)$ varies linearly as a function of the applied voltage. According to Eq. (1), the respective slope parameter gives the ideality factor and the extrapolation to zero applied voltage gives the zero-bias barrier height. With the effective Richardson constant $A_R^{**}=112$ A $cm^{-2}$ $K^{-2}$ (Ref. 21) and the diode area $A=7.85\times10^{-3}$ $cm^2$ we obtained an effective barrier height $\Phi_{B0}^{eff}=0.62$ eV and an ideality factor $n=1.41$. The homogeneous and the effective barrier heights of this Sn/Si(111) contact thus differ by $\Phi_{B0}-\Phi_{B0}^{eff}=0.059$ eV.

Effective Schottky barrier heights and ideality factors vary from diode to diode, therefore, it is common practice to take averages. Figure 2 displays histograms of the effective barrier heights and ideality factors for as many as 38 Sn/Si(111) Schottky contacts. The statistical analysis yields the mean effective barrier height $\langle\Phi_{B0}^{eff}\rangle=(0.64\pm0.017)$ eV and the mean ideality factor $\langle n\rangle=1.22\pm0.09$. Such mean values disregard the pronounced correlation between effective barrier heights and ideality factors.

Figure 3 now displays the effective barrier heights of the same 38 diodes as a function of their ideality factors. We would like to emphasize that the barrier heights plotted in

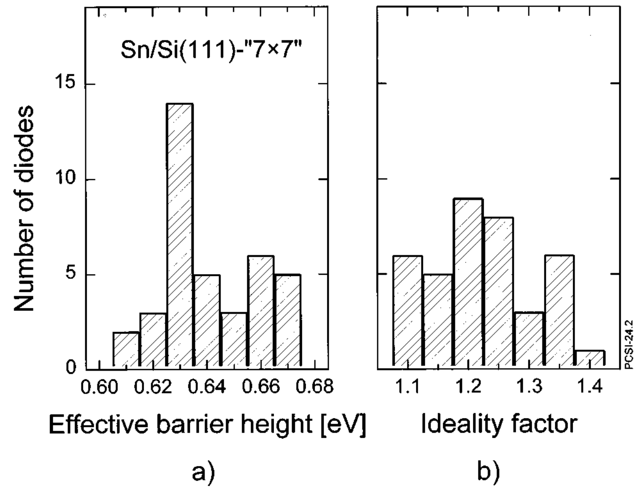


FIG. 2. Effective Schottky barrier heights (a) and ideality factors (b) obtained from $I$-$V$ characteristics of 38 Sn/Si(111)-"7×7" diodes. The mean values of the effective barrier heights and of the ideality factors are $\langle\Phi_{B0}^{eff}\rangle=0.64$ eV and $\langle n\rangle=1.22$, respectively.

Figs. 2 and 3 result from the standard evaluation of the experimental $I$-$V$ curves using Eq. (1) rather than from fitting procedures employing Eq. (4). Figure 3 clearly confirms the well-known linear correlation[8,11] between effective barrier heights and ideality factors. In general, large effective barrier heights are related with small and then close to unity ideality factors. This trend may be understood in terms of nonuniform interfaces.

Both the ideality factor and the effective barrier heights depend, in a complicated way, on the patch density and the standard deviation of the patch-parameter. Due to the implicit form of Eq. (4), there is no analytic expression available. Therefore, we performed a numerical simulation of the effective barrier height and the ideality factor as a function of the patch density for different standard deviations of the patch-parameter. The calculation procedure was as follows. With the parameters chosen we first calculated $I$-$V$ curves using Eq. (4). We then applied the standard evaluation pro-

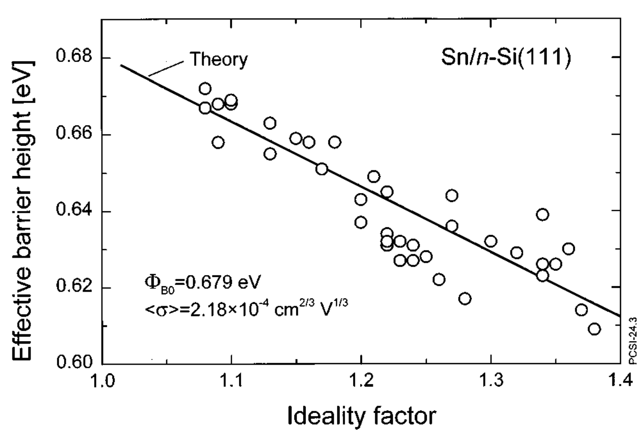


FIG. 3. Effective barrier heights of Sn/Si(111)-"7×7" diodes as a function of their ideality factors at room temperature. The data are the same as in Fig. 2. The full line is the result of a numerical simulation.

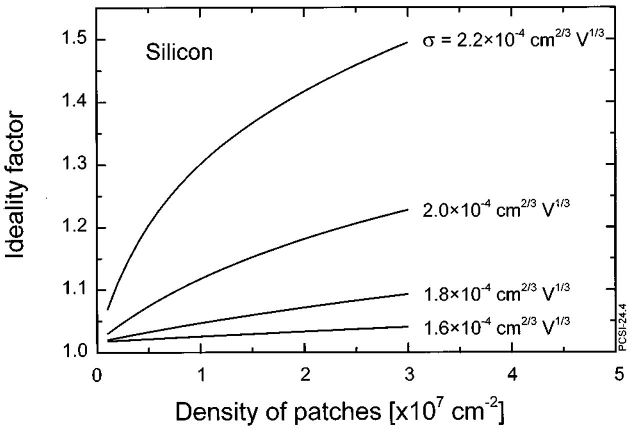


FIG. 4. Simulation of the ideality factor as a function of the patch density for four different standard deviations $\sigma$ of the patch parameter $\gamma$. The silicon contact was assumed to have a homogeneous barrier height $\Phi_{B0}=0.679$ eV and a series resistance $R_s=80\ \Omega$ and the doping density of the substrate was set to $N_d=1.4\times10^{15}\ \mathrm{cm}^{-3}$.

cedure using Eq. (1) to these calculated $I$-$V$ curves and obtained effective barrier heights and ideality factors. Figure 4 displays our results for the ideality factors. As one might intuitively expect, the larger the patch density and/or the standard deviation of the patch-parameter, the larger the respective ideality factor. Therefore, the ideality factors represent a direct measure of the interface uniformity. This finding and the assumption that the patches have smaller barrier heights than the homogeneous contact explains the experimentally observed reduction of the barrier heights with increasing ideality factors.

The full line in Fig. 3 shows the effective barrier as a function of the ideality factor which were both obtained from our simulations as described in the preceding paragraph. The parameters used were a homogeneous barrier height $\Phi_{B0}=0.679$ eV, a series resistance $R_s=90\ \Omega$, and a standard variation of the patch parameter $\sigma=2.18\times10^{-4}\ \mathrm{cm}^{2/3}\ \mathrm{V}^{1/3}$. This choice was motivated by the parameters obtained from the fit of Eq. (4) to the experimental data displayed in Fig. 1. The patch density $\rho_p$ increased up to about $2\times10^7\ \mathrm{cm}^{-2}$. The result of our simulations is indeed a straight line. It is worth mentioning that a ''simple'' linear regression of the experimental data yields the same straight line and, as a consequence, the same homogeneous barrier height. This finding confirms our earlier conclusion that homogeneous barrier heights may be obtained by linear extrapolations of $\Phi_{B0}^{\mathrm{eff}}$ vs $n$ plots to $n=n_{if}=1.01\div1.03$, the image-force-controlled ideality factor of homogeneous Schottky contacts. This procedure is much easier than the determination of the homogeneous barrier heights by fitting the complicated Eq. (4) to many experimental $I$-$V$ curves.

In our numerical simulations we made the simplifying assumption that all diodes are characterized by one and the same standard deviation $\sigma$ of the patch-parameter. Actually, the standard deviation of the patch-parameter may vary from diode to diode. This might explain the scatter of the experimental data around the straight line in Fig. 3.

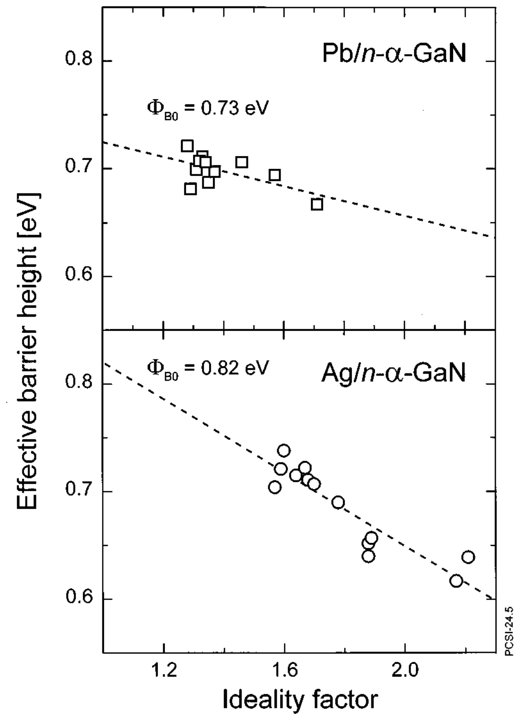


FIG. 5. Effective barrier heights of Pb- and Ag/$n$-GaN(0001) diodes as a function of their ideality factors at room temperature. The dashed lines are linear least-squares fits to the experimental data.

Linear correlations between effective Schottky barrier heights and ideality factors were also observed for a number of other metal-semiconductor combinations.[8,11] As examples, results of Ag/Si(111) and Ag as well as Pb/GaN(0001) Schottky contacts are displayed in Figs. 5 and 6. The data of the GaN Schottky contacts clearly show the importance of $\Phi_{B0}^{\mathrm{eff}}$ vs $n$ plots. Figure 5 gives the Schottky barrier heights of homogeneous Pb and Ag/GaN contacts as 0.73 and 0.82 eV, respectively. The simple statistical analysis of the data, on the other hand, yields *mean* effective barrier heights of 0.70 and 0.69 eV, respectively. The mean effective and the homogeneous Schottky barrier heights of the Ag/GaN contacts

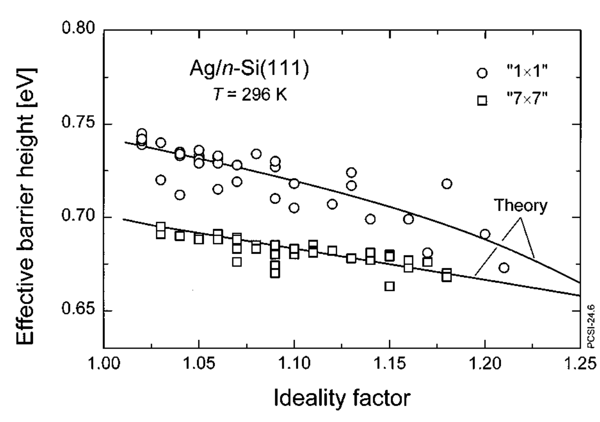


FIG. 6. Effective barrier heights of Ag/Si(111)-''7×7''and -1×1 diodes as a function of their respective ideality factors at room temperature. The full lines are results of numerical simulations.

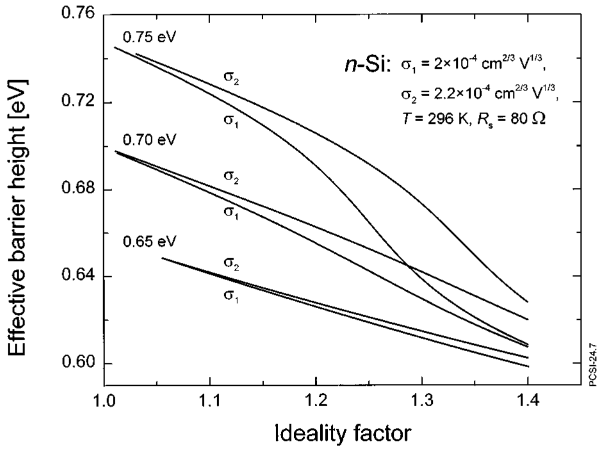


FIG. 7. Simulation of the effective barrier height as a function of the ideality factor for three different homogeneous barrier heights and two different standard deviations each of the patch parameter. The silicon substrate was assumed to have a doping density $N_d = 1.4\times10^{15}$ cm$^{-3}$ and a series resistance $R_s = 80$ Ω.

differ by as much as 130 meV. This large discrepancy is obviously caused by the large ideality factors of the Ag/GaN diodes. They might be a consequence of the poor quality of the GaN epilayers used.

Effective Schottky barrier heights will always decrease as a function of the ideality factors. However, whether the correlation is linear depends on the actual inhomogeneities. A best fit to the Ag/Si(111)-''7×7'' data of Fig. 6 is achieved with $\Phi_{B0} = 0.70$ eV and $\sigma = 2.35\times10^{-4}$ cm$^{2/3}$ V$^{1/3}$ and gives a strict linear correlation. The Ag/Si(111)-''1×1'' data, on the other hand, are best described by the parameters $\Phi_{B0} = 0.745$ eV and $\sigma = 2.012\times10^{-4}$ cm$^{2/3}$ V$^{1/3}$. The fit is linear up to $n \approx 1.15$ and is slightly bent above this value. Such nonlinearities will be discussed by considering further results of the numerical simulations outlined above.

Figure 7 shows $\Phi_{B0}^{\mathrm{eff}}$ vs $n$ plots for three different homogeneous Schottky barrier heights and two different standard deviations of the patch parameter each. The $\Phi_{B0}^{\mathrm{eff}}(n)$ curves become nonlinear above $n \approx 1.2$ for large effective barrier heights and small standard deviations of the patch-parameter. The curves may be divided into three regions. First, the correlation is close to linear for ideality factors near to unity. In the second region, the curve exhibits a strong downward bent. It is eventually followed by a third and almost linear part for large ideality factors. In this third region the patch density becomes large. Then, the effective barrier height of the contact is almost completely controlled by the patches and the homogeneous Schottky barrier height is of less importance. Therefore, some care must be taken if experimental data are analyzed in terms of $\Phi_{B0}^{\mathrm{eff}}(n)$ plots and the ideality factors are large. In such cases a detailed analysis of individual $I$-$V$ characteristics using Eq. (4) should be carried out. However, this procedure requires the input of material parameters such as the modified Richardson constant, the exact doping density, the dielectric constant and the density of states in the majority-carrier band of the semiconductor. If these parameters are not available—as in the case of GaN—then the extrapolation of the effective barrier heights to $n = n_{if} \approx 1$ should be used as a first-order approximation. At present, we cannot derive an analytic relation for the ideality-factor range in which $\Phi_{B0}^{\mathrm{eff}}$ vs $n$ plots are linear. This needs further investigation.

## V. CONCLUSIONS

It is common practice to determine effective Schottky barrier heights and ideality factors from $I$-$V$ characteristics of real metal-semiconductor contacts using the $I$-$V$ relationship derived for thermionic transport across laterally uniform interfaces. Both effective barrier heights and ideality factors vary from diode to diode. However, we found pronounced correlations between the effective barrier heights and the ideality factors and attributed this behavior to local deviations of the barrier height from the value characteristic of uniform interfaces. The homogeneous Schottky barrier height of metal-semiconductor contacts may be easily obtained from plots of the effective barrier heights of a number of contacts versus their ideality factors. *If* such plots may be fitted by straight lines, then the extrapolation to the ideality factor $n = n_{if} \approx 1$ directly gives the homogeneous Schottky barrier height. We justify this procedure by numerical simulations of $I$-$V$ curves which use Tung's theory of laterally inhomogeneous contacts with Gaussian distributions of the parameter characterizing such patchy metal-semiconductor interfaces. These homogeneous barrier heights rather than effective barrier heights of individual contacts or mean values should be used to discuss theories on the physical mechanisms that determine the barrier heights of metal-semiconductor contacts. Provided the semiconductor substrate is well characterized then the homogeneous Schottky barrier height may be obtained from the $I$-$V$ characteristic of even one contact.

## ACKNOWLEDGMENT

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