

The double Gaussian distribution of barrier heights in Au/*n*-GaAs Schottky diodes from I – V – T characteristics

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Abstract

The current–voltage (I – V) and capacitance–voltage (C – V) characteristics of Au/*n*-GaAs contacts have been measured in the temperature range of 80–300 K. An abnormal decrease in the experimental BH Φ_b and an increase in the ideality factor n with a decrease in temperature have been observed. This behaviour has been attributed to the barrier inhomogeneities by assuming a Gaussian distribution of barrier heights at the metal–semiconductor interface. The temperature-dependent I – V characteristics of the Au/*n*-GaAs contact have shown a double Gaussian distribution giving mean barrier heights of 0.967 and 0.710 eV and standard deviations of 0.105 and 0.071 V, respectively. A modified $\ln(I_0/T^2) - q^2\sigma_s^2/2k^2T^2$ versus $1/T$ plot for the two temperature regions then gives $\bar{\Phi}_{b0}$ and A^* as 0.976 and 0.703 eV, and 13.376 and 8.110 A cm^{−2} K^{−2}, respectively. Furthermore, a value of -0.674 meV K^{−1} for the temperature coefficient has been obtained, and the value of -0.674 meV K^{−1} for the Au/*n*-GaAs Schottky diode is in close agreement with those in the literature.

1. Introduction

Due to the technological importance of Schottky barrier diodes (SBDs) which are the simplest of the MS (metal–semiconductor) contact devices, a full understanding of the nature of their electrical characteristics is of greater interest [1–5]. It is well known that interface properties of the MS contacts have a dominant influence on the device performance, reliability and stability [1–11]. Schottky barrier inhomogeneity at MS interfaces has been considered as an important factor in explaining the non-ideal behaviour of the Schottky diodes and the dependence of the SB (Schottky barrier) values on the doping level and used measurement methods [4–13]. The ballistic electron emission microscopy (BEEM) has also supported the existence of a Gaussian distribution of barrier heights (BHs) in Schottky diodes [14–17]. The electrical behaviour of semiconductor/metal contacts having spatially inhomogeneous barrier heights has attracted much theoretical [4–15], computational [4–22] and experimental [7–30] attention indicating that the current

density through small, low barrier height regions on the surface of an otherwise high barrier height semiconductor/metal contact should be a strong function of the spatial dimensions of the low barrier height regions.

Schottky diodes with low BH have found applications in devices operating at cryogenic temperatures such as infrared detectors, sensors in thermal imaging, microwave diodes, gates of transistors and infrared and nuclear particle detectors [1–3, 9–11]. Therefore, analysis of the current voltage (I – V) characteristics of the SBDs at room temperature only does not give detailed information about their conduction process or the nature of barrier formation at the MS interface [5–11]. The temperature dependence of the I – V characteristics allows us to understand different aspects of conduction mechanisms [5–15]. Analysis of the I – V characteristics of SBDs based on thermionic emission theory usually reveals an abnormal decrease in the SBH Φ_b and an increase in the ideality factor n with a decrease in temperature [18–30]. The decrease in the BH at low temperatures leads to nonlinearity in the activation energy $\ln(I_0/T^2)$ versus $1/T$ plot. These findings

have been satisfactorily explained recently by incorporating the concept of barrier inhomogeneities and introducing a thermionic emission mechanism with a Gaussian distribution function with a mean BH and a standard deviation for the description in some studies [6–12, 18–30].

In the present study, the *I*–*V* and capacitance–voltage (*C*–*V*) characteristics of Au Schottky contacts on an *n*-GaAs substrate were measured over the temperature range of 80–300 K. The temperature-dependent barrier characteristics of the Au/*n*-GaAs Schottky contacts were interpreted by assuming a Gaussian spatial distribution of barrier height.

2. Experimental procedure

The samples have been prepared using cleaned and polished *n*-GaAs (as received from the manufacturer) with (100) orientation and $2\text{--}5 \times 10^{17} \text{ cm}^{-3}$ carrier concentrations. Before making contacts, the *n*-GaAs wafer was dipped in $5\text{H}_2\text{SO}_4 + \text{H}_2\text{O}_2 + \text{H}_2\text{O}$ solution for 1.0 min to remove the surface damage layer and undesirable impurities and then in $\text{H}_2\text{O} + \text{HCl}$ solution and then followed by a rinse in deionized water of 18 MΩ. The wafer has been dried with high-purity nitrogen and inserted into the deposition chamber immediately after the etching process. Au–Ge (88%, 12%) for ohmic contacts was evaporated on the back of the wafer in a vacuum-coating unit of 10^{-5} Torr. Then, a low resistance ohmic contact was formed by thermal annealing at 450 °C for 3 min when N_2 is passed through a quartz tube furnace. The Schottky contacts have been formed by evaporating Au as dots with a diameter of about 1.35 mm on the front surface of *n*-GaAs. The *I*–*V* characteristics of the devices were measured in the temperature range of 80–300 K using a temperature-controlled JANES vpf-475 cryostat, which enables us to make measurements in the temperature range of 77–450 K, and a Keithly 220 programmable constant current source and a Keithly 199 dmm/scanner under dark conditions. The capacitance–voltage (*C*–*V*) measurements were performed using an HP 4192A LF impedance analyser. The sample temperature was always monitored by using a copper–constantan thermocouple and a LAKESHORE 321 auto-tuning temperature controller with sensitivity better than ± 0.1 K.

3. Results and discussion

The electrical *I*–*V* and *C*–*V* measurements of the device were made in the temperature range of 80–300 K. The current through a uniform metal–semiconductor interface due to thermionic emission can be expressed as [1]

$$I = I_0 \exp\left(\frac{qV}{nkT}\right) \left[1 - \exp\left(-\frac{qV}{kT}\right)\right], \quad (1)$$

where I_0 is the saturation current derived from the straight line intercept of $\ln I$ at $V = 0$ and is given by

$$I_0 = AA^*T^2 \exp\left(-\frac{q\Phi_{\text{ap}}}{kT}\right), \quad (2)$$

where q is the electron charge, V is the forward-bias voltage, A is the effective diode area, k is the Boltzmann constant, T is the absolute temperature, A^* is the effective Richardson constant of $8.16 \text{ A cm}^{-2} \text{ K}^{-2}$ for *n*-type GaAs, Φ_{ap} is the zero-bias

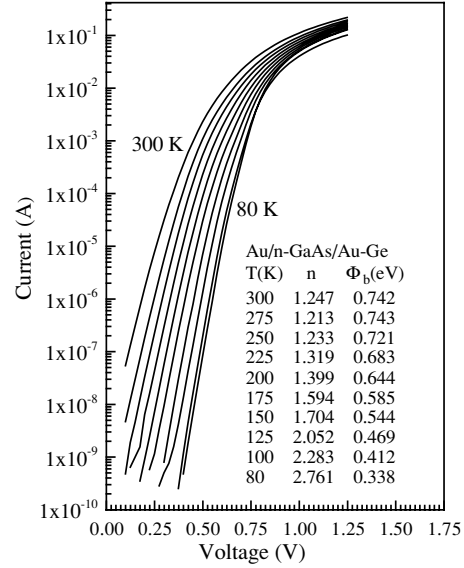


Figure 1. Experimental forward-bias current–voltage characteristics of a typical Au/*n*-GaAs/Au-Ge Schottky contact in the temperature range of 80–300 K.

apparent BH and n is the ideality factor. From equation (1), the ideality factor n can be written as

$$n = \frac{q}{kT} \left(\frac{dV}{d \ln I} \right). \quad (3)$$

The ideality factor, n , is introduced to take into account the deviation of the experimental *I*–*V* data from the ideal thermionic model and should be $n = 1$ for an ideal contact.

The decrease in the BH with a decrease in temperature can be explained by the lateral distribution of BH if the barrier height has a Gaussian distribution of the BHs over the Schottky contact area with the mean BH Φ_b and standard deviation σ_s . The standard deviation is a measure of the barrier homogeneity. The Gaussian distribution of the BHs yields the following expression for the BH [7–10]:

$$\Phi_{\text{ap}} = \Phi_b - \frac{q\sigma_s^2}{2kT}, \quad (4)$$

where Φ_{ap} is the apparent BH measured experimentally. The temperature dependence of σ_s is usually small and can be neglected. The observed variation of the ideality factor with temperature in the model is given by [8]

$$\left(\frac{1}{n_{\text{ap}}} - 1 \right) = -\rho_2 + \frac{q\rho_3}{2kT}, \quad (5)$$

where n_{ap} is the apparent ideality factor and ρ_2 and ρ_3 quantify the voltage deformation of the BH distribution.

Figure 1 shows the semilog forward-bias *I*–*V* characteristics of the Au/*n*-GaAs Schottky contact in the temperature range of 80–300 K. The *I*–*V* plots shift towards the higher bias side with decrease in temperature. The experimental values of the barrier height Φ_{ap} and the ideality factor n for the device were determined from intercepts and slopes of the forward-bias $\ln I$ versus V plot at each temperature, respectively. The experimental values of Φ_{ap} and n range from 0.742 eV and 1.247 (at 300 K) to 0.338 eV and 2.761 (at 80 K), respectively. Figure 2 (indicated by closed

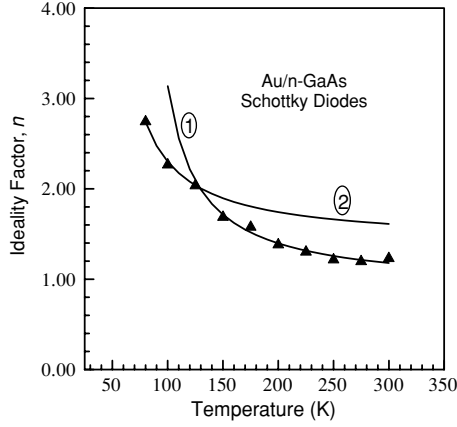


Figure 2. Temperature dependence of the ideality factor for the Au/*n*-GaAs Schottky contact (the filled triangles). The continuous curves show estimated values of the ideality factor using equation (5) for two Gaussian distributions of barrier heights with $\rho_2 = -0.113$, $\rho_3 = -0.0137$ V at 125–300 K (curve 1) and $\rho_2 = 0.287$, $\rho_3 = -0.0048$ V at 80–125 K (curve 2).

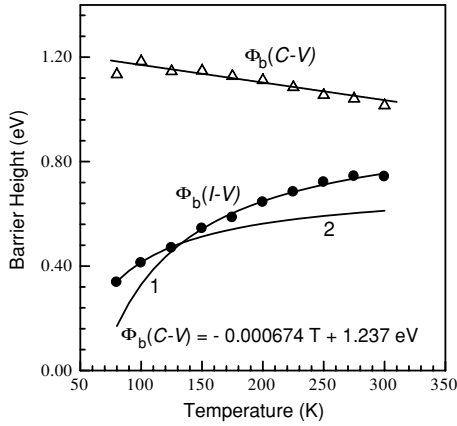


Figure 3. Temperature dependence of the experimental zero-bias barrier height (the filled circles) and for the Au/*n*-GaAs Schottky contact and *C*–*V* barrier height (the open triangles). The continuous curve related to the filled circles represents estimated values of Φ_{ap} using equation (4) for two Gaussian distributions of barrier heights with $\Phi_{b0} = 0.967$ eV and $\sigma_s = 0.105$ V at 125–300 K (curve 1) and $\Phi_{b0} = 0.710$ eV and $\sigma_s = 0.071$ V at 80–125 K (curve 1).

triangles) shows the values of n as a function of temperature. The experimental value of n increased with a decrease in temperature, as can be seen in figure 2. The experimental values of Φ_{ap} (indicated by closed circles in figure 3) as a function of the temperature decreased with a decrease in temperature.

Furthermore, the BH Φ_{C-V} values at various temperatures for the Au/*n*-GaAs Schottky diode have been calculated from its experimental reverse bias C^{-2} –*V* characteristics given in figure 4. The experimental values of Φ_{C-V} as a function of the temperature are indicated by open triangles in figure 3; these values increased with a decrease in temperature. The experimental values of Φ_{C-V} range from 1.021 eV at 300 K to 1.140 eV at 80 K. As can be seen, the C^{-2} –*V* curve gave BH values higher than those derived from *I*–*V* measurements as expected. We will return to this point later. The experimental Φ_{C-V} versus *T* plot yields the values of $\Phi_{C-V}(T=0) = 1.237$ eV

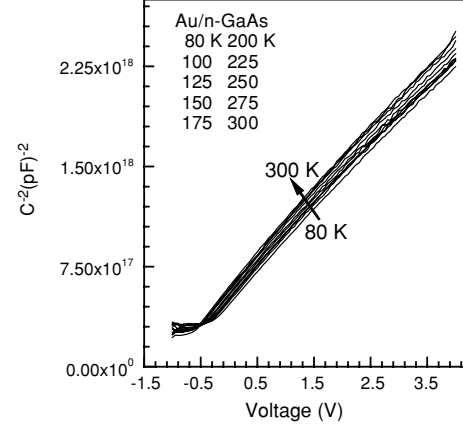


Figure 4. Experimental capacitance–voltage characteristics of a typical Au/*n*-GaAs/Au-Ge Schottky contact in the temperature range of 80–300 K.

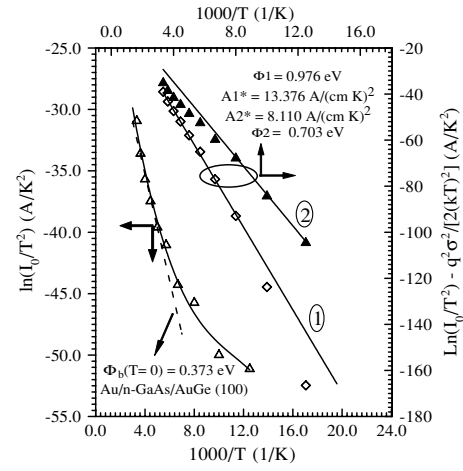


Figure 5. Richardson plot of the $\ln(I_0/T^2)$ versus $1/T$ plot (the open triangles) and modified Richardson $\ln(I_0/T^2) - q^2\sigma_s^2/2k^2T^2$ versus $1/T$ plot for the Au/*n*-GaAs (100) Schottky contact according to two Gaussian distributions of barrier heights. The filled triangles represent the plot calculated for $\sigma_s = 0.071$ V and the open squares represent the plot calculated for $\sigma_s = 0.105$ V. The straight lines 1 and 2 indicate the best fitting of the data in temperature ranges of 125–300 K and 80–125 K.

for the BH and $\alpha = -0.674$ meV K^{−1} for the BH temperature coefficient.

Figure 5 (indicated by open triangles) shows a conventional activation energy $\ln(I_0/T^2)$ versus $1/T$ plot according to equation (2). An experimental $\ln(I_0/T^2)$ versus $1/T$ plot should yield a straight line with a slope given by a BH at 0 K, $\Phi_{b0}(T=0)$. The experimental data are seen to fit asymptotically to a straight line at higher temperatures only. An activation energy value of 0.373 eV from the slope of this straight line was obtained for the device. Bowing of the experimental $\ln(I_0/T^2)$ versus $1/T$ curve is caused by the temperature dependence of the BH and ideality factor due to the existence of the surface inhomogeneities of the GaAs substrate [5–11]. As will be discussed below, the deviation in the Richardson plots may be due to the spatially inhomogeneous BHs and potential fluctuations at the interface that consist of low and high barrier areas [5–13], that is, the

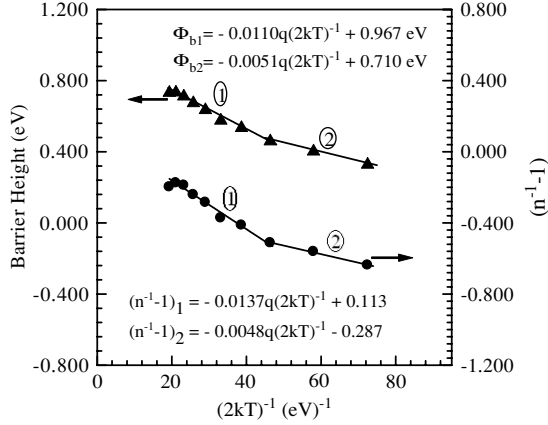


Figure 6. Zero-bias apparent barrier height (the filled triangles) and ideality factor (the filled circles) versus $1/(2kT)$ curves of the Au/*n*-GaAs Schottky contact according to two Gaussian distributions of BHs. The data show linear variation in the two temperature ranges with a transition around 125 K.

current through the diode will flow preferentially through the lower barriers in the potential distribution. As explained in [6, 11, 27], since current transport across the MS interface is a temperature-activated process, at low temperatures, current transport will be dominated by the current flowing through the patches of lower SBH and larger ideality factor. As the temperature increases, the dominant BH will increase with the temperature and bias voltage [6, 11, 27]. Thereby, the commonly observed deviation from classical thermionic emission theory can be explained by a recent model based on the assumption of a spatial fluctuation of the BH at interface. That is, the observed changes depending on temperature may be interpreted satisfactorily by incorporation of the concept of barrier inhomogeneities into thermionic emission theory [5–12, 18–23, 25–30].

Moreover, the difference between the measured *I*–*V* and *C*–*V* SBH in the metal/semiconductor is also evidence for Schottky BH inhomogeneity. The reason for the discrepancy between the *I*–*V* and *C*–*V* measured SBH is clear. The current in the *I*–*V* measurement is dominated by the current which flows through the region of low SBH. The measured *I*–*V* BH is significantly lower than the weighted arithmetic average of the SBHs. On the other hand, the *C*–*V* measured BH is influenced by the distribution of charge at the depletion region boundary and this charge distribution follows the weighted arithmetic average of the SBH inhomogeneity; hence the BH determined by *C*–*V* is close to the weighted arithmetic average of the SBHs. Therefore, the SBH determined from the zero-bias intercept assuming thermionic emission as current transport mechanism is well below the *C*–*V* measured BH and the weighted arithmetic average of the SBHs [5, 8, 31].

The continuous curves in figures 2 and 3 and the linearity of the apparent barrier height or ideality factor versus $1/T$ curves in figure 6 show that the temperature dependence experimental data of the Au/*n*-GaAs (100) Schottky contact are in agreement with the recent model which is related to thermionic emission over a Gaussian BH distribution [7–12, 18–23]. Fitting of the experimental *I*–*V* data to equations (2) and (3) gives Φ_{ap} and n_{ap} , respectively, which should obey

equations (4) and (5). Thus, the plot of Φ_{ap} versus $1/T$ (figure 6) should be a straight line with the intercept at the ordinate determining the zero-bias mean BH Φ_{b0} and the slope giving the zero-bias standard deviation σ_s . The experimental Φ_{ap} versus $1/T$ and n_{ap} versus $1/T$ plots (figure 6) drawn by means of the data obtained from figure 1 respond to two lines instead of a single straight line with transition occurring at 125 K. The above observations indicate the presence of two Gaussian distributions of barrier heights in the contact area. The intercepts and slopes of these straight lines give two sets of values of Φ_{b0} and σ_s as 0.967 and 0.105 V in the temperature range of 125–300 K (distribution 1), and as 0.710 eV and 0.071 V in the temperature range of 80–125 K (distribution 2). Furthermore, as can be seen in figure 3, the Φ_{ap} values estimated from equation (4) over the entire temperature range of 80–300 K using Φ_{b0} and σ_s are shown by the continuous curves 1 and 2. That is, the continuous solid lines related to the filled circles in figure 3 represent the data estimated with these parameters using equation (4).

The existence of a double Gaussian on Au/*n*-GaAs Schottky diodes was already experimentally proven by BEEM [17]. These changes were ascribed to the chemical treatment of the GaAs surface by Vanalme *et al* [17]. Likewise, as indicated also by Chand and Kumar [10], the existence of a double Gaussian in the metal/semiconductor contacts can be attributed to the nature of the inhomogeneities themselves in the two cases. This may involve variation in the interface composition/phase, interface quality, electrical charges, nonstoichiometry, etc. Further, such inhomogeneities might occur on a scale that inhibits their detection by the usual characterization tools. They are important enough to electrically influence the *I*–*V* characteristics of the Schottky diodes, at particularly low temperatures. Thus, *I*–*V* measurements at very low temperatures are capable of revealing the nature of barrier inhomogeneities present in the contact area. That is, the existence of a second Gaussian distribution at very low temperatures may possibly arise due to some phase change taking place on cooling below a certain temperature. Furthermore, the temperature range covered by each straight line suggests the regime where the corresponding distribution is effective.

Similarly, the plot of n_{ap} versus $1/T$ should also possess different characteristics in the two temperature ranges because the diode contains two barrier height distributions. This can be clearly seen in figure 6. The intercept and slope of the straight lines in n_{ap} versus $1/T$ plot give the voltage coefficients ρ_2 and ρ_3 , respectively. The values of ρ_2 obtained from the intercepts of the experimental n_{ap} versus $1/T$ plot (figure 6) are –0.113 in 125–300 K range (distribution 1) and 0.287 in 80–125 K range (distribution 2), whereas the values of ρ_3 from the slopes are –0.0137 V in 125–300 K range and –0.0048 in 80–125 K range. The linear behaviour of this plot demonstrates that the ideality factor does indeed express the voltage deformation of the Gaussian distribution of the Schottky BH. The continuous solid lines in figure 2 represent data estimated with the above values of ρ_2 and ρ_3 using equation (5). As can be seen, the computed values exactly coincide with the experimental results in the respective temperature ranges for two different distributions. As can be seen from the n_{ap} versus $1/T$ plot, ρ_3 value or the slope of distribution 1 is larger than that of

distribution 2; therefore we may point out that distribution 1 is a wider and relatively higher barrier height with bias coefficients ρ_2 and ρ_3 being smaller and larger, respectively. Thus, we can say that distribution 2 at very low temperatures may possibly arise due to some phase change taking place on cooling below a certain temperature.

Furthermore, as mentioned above, the conventional activation energy $\ln(I_0/T^2)$ versus $1/T$ plot has showed nonlinearity at low temperatures. To explain these discrepancies, using $\bar{\Phi}_{b0}$ in place of the apparent BH Φ_{ap} in equation (2) and combining equations (2) and (4) according to the Gaussian distribution of the BH, it can be rewritten as

$$\ln\left(\frac{I_0}{T^2}\right) - \left(\frac{q^2\sigma_s^2}{2k^2T^2}\right) = \ln(AA^*) - \frac{q\bar{\Phi}_{b0}}{kT} \quad (6)$$

and a modified activation energy plot from this expression is obtained. Using the experimental I_0 data, a modified $\ln(I_0/T^2) - q^2\sigma_s^2/2k^2T^2$ versus $1/T$ plot can be obtained according to equation (6) and should give a straight line with slope directly yielding the mean $\bar{\Phi}_{b0}$ and the intercept ($= \ln AA^*$) at the ordinate determining A^* for a given diode area A . The $\ln(I_0/T^2) - q^2\sigma_s^2/2k^2T^2$ values were calculated for both values of σ obtained for the temperature ranges of 80–125 K and 125–300 K. Thus, the closed triangles and open squares in figure 5 have given the modified $\ln(I_0/T^2) - q^2\sigma_s^2/2k^2T^2$ versus $1/T$ plots for both values of σ . The best linear fitting to these modified experimental data is depicted by solid lines in figure 5 which represent the true activation energy plots in respective temperature ranges, yielding zero-bias mean BH $\bar{\Phi}_{b0}$ of 0.703 eV (in the range of 80–125 K) and 0.976 eV (in the range of 125–300 K). These values match exactly with the mean BHs obtained from the Φ_{ap} versus $1/T$ plot in figure 6. Likewise, the mean BH values from figures 5 and 6 in high temperature range are very close to the BH values from C^{-2} - V characteristics. This indicates that the BH measured by C - V is always close to the weighted arithmetic average of the SBHs in the inhomogeneous MS contacts. The intercepts at the ordinate give the Richardson constant A^* as $8.110 \text{ A cm}^{-2} \text{ K}^{-2}$ (in 80–125 K range) and $13.376 \text{ A cm}^{-2} \text{ K}^{-2}$ (in 125–300 K range) without using the temperature coefficient of the BHs. The Richardson constant value of $8.110 \text{ A cm}^{-2} \text{ K}^{-2}$ for the range of 80–125 K is almost the same with a value of $8.16 \text{ A cm}^{-2} \text{ K}^{-2}$ known for electrons in n -type GaAs.

4. Conclusion

The above results suggest that the experimental data of the present Au/ n -GaAs Schottky diode can be satisfactorily explained by assuming the existence of two Gaussian distributions of the Schottky barrier heights in the temperature range of 80–300 K, suggesting that the contacts are not spatially uniform. The temperature range covered by each straight line suggests the regime where the corresponding distribution is effective. That is, the Φ_{ap} versus $1/T$ plot of ideal Schottky diodes (homogeneous contact) should give a horizontal line while this plot for a spatially uniform contact expressed by a Gaussian distribution of BHs has a straight line

with negative slope, or two straight lines with negative slope for double Gaussian distribution of BHs as in the present case. The same has been also observed for n_{ap} versus $1/T$ plot as in the present case.

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