The Schottky Conjecture and beyond

Debabrata Biswas\textsuperscript{1,2}

\textsuperscript{1}Bhabha Atomic Research Centre, Mumbai 400 085, INDIA
\textsuperscript{2}Homi Bhabha National Institute, Mumbai 400 094, INDIA

The ‘Schottky Conjecture’ deals with the electrostatic field enhancement at the tip of compound structures such as a hemiellipsoid on top of a hemisphere. For such a 2-primitive compound structure, the apex field enhancement factor $\gamma_a$ is conjectured to be multiplicative ($\gamma_a = \gamma_a^{(1)} \gamma_a^{(2)}$) provided the structure at the base (labelled 1, e.g. the hemisphere) is much larger than the structure on top (referred to as crown and labelled 2, e.g. the hemi-ellipsoid). We first demonstrate numerically that for generic smooth structures, the conjecture holds in the limiting sense when the apex radius of curvature of the primitive-base $R_a^{(1)}$, is much larger than the height of the crown $h_2$ (i.e. $h_2/R_a^{(1)} \rightarrow 0$). If the condition is somewhat relaxed, we show that it is the electric field above the primitive-base (i.e. in the absence of the crown), averaged over the height of the crown, that gets magnified instead of the field at the apex of the primitive-base. This observation leads to the Corrected Schottky Conjecture (CSC), which for 2-primitive structures reads as $\gamma_a \simeq \langle \gamma_a^{(1)} \rangle \gamma_a^{(2)}$ where $\langle \cdot \rangle$ denotes the average value over the height of the crown. For small protrusions ($h_2/h_1$ typically less than 0.2), $\langle \gamma_a^{(1)} \rangle$ can be approximately determined using the Line Charge Model so that $\gamma_a^{(1)} \simeq \gamma_a^{(2)} (2R_a^{(1)}/h_2) \ln(1+h_2/2R_a^{(1)})$. The error is found to be within 1% for $h_2/R_a^{(1)} < 0.05$, increasing to about 3% (or less) for $h_2/R_a^{(1)} = 0.1$ and bounded below 5% for $h_2/R_a^{(1)}$ as large as 0.5. The CSC is also found to give good results for 3-primitive compound structures. The relevance of the Corrected Schottky Conjecture for field emission is discussed.

I. INTRODUCTION

In 1923, Schottky argued that the apex field enhancement factor (AFEF) at the tip of a compound structure should be a product of the AFEF values of the successive primitive structures comprising it, provided each structure is much smaller than the preceding one\textsuperscript{[12]}. Nearly a hundred years since, there is renewed interest\textsuperscript{[13,14]} in this conjecture for various reasons. A primary cause of breakdown in vacuum devices is thought to be electron emission from micro-protrusions on an otherwise smooth surface on application of a DC or RF field. Since, appreciable electron emission requires electric field strengths upwards of 3GV/m, it is now accepted that micro-protrusions can have very high field enhancement factors due to the compounding effect suggested by Schottky\textsuperscript{[1]}\textsuperscript{11}. The conjecture is also relevant in situations where field emission is desirable since, even though we now have a fair idea about the field enhancement factor of generic single primitive structures\textsuperscript{[11,12]}, a simple and useful model of compound structures is yet to be formulated. An analytical formula (even an empirical one) for the AFEF of compound structures would no doubt be extremely useful in optimizing the field emission current with respect to the parameters of single emitters and might well be of future use in studying large area field emitters\textsuperscript{[15,16]} of compound entities. It is thus necessary that we revisit the Schottky Conjecture (SC) using the tools presently at our disposal and try to go beyond in situations that do not quite obey the stringent requirements of the conjecture.

The apex field enhancement factor $\gamma_a$ is defined as the ratio of the local field at the apex ($E_a$) and the macroscopic field far away from the emitter ($E_0$). In a planar diode configuration with the cathode plate at $z = 0$ and the anode plate at $z = D$ having a potential difference $V$ with respect to the cathode plate, the macroscopic field $E_0 = V/D$. Consider now an axially symmetric curved emitter of height $h$ (with $h << D$) and apex radius of curvature $R_a$ placed normal to the cathode plate. The local field at the apex $E_a = \gamma_a E_0$ where $\gamma_a$ is the apex field enhancement factor of an isolated emitter with the anode far away\textsuperscript{[14]}

Consider now two structures having AFEF $\gamma_a^{(1)}$ and $\gamma_a^{(2)}$ respectively. When the second structure is mounted on top of the first, the compound structure does not necessarily have its AFEF value as $\gamma_a^{(1)} \gamma_a^{(2)}$. However, if the apex radius of curvature of the first structure $R_a^{(1)}$ is much larger compared to the height $h_2$ of the second structure, the AFEF of the compound structure can be closely approximated by $\gamma_a^{(1)} \gamma_a^{(2)}$ since the second structure finds itself on a quasi-planar base and takes advantage of the enhanced local field near the apex of the first structure. Thus, at a basic level, the Schottky Conjecture seems plausible provided $h_2/R_a^{(1)} \rightarrow 0$. If the system has more than 2 primitive structures, a similar logic would imply that the AFEF of the compound structure be a product of the primitive AFEF values provided $h_{i+1}/R_a^{(i)} \rightarrow 0$ for all $i$. Thus the AFEF value of the compound structure having $N$ primitives may be expressed as $\gamma_a^{(C)} = \prod_{i=1}^{N} \gamma_a^{(i)}$.

In practice, compound structures may have $h_{i+1}/R_a^{(i)}$ small but non-zero and it would be desirable in such cases to have a Corrected Schottky Conjecture with correction terms\textsuperscript{[15]} expressed in terms of $h_{i+1}/R_a^{(i)}$. In other situations, $h_{i+1}/R_a^{(i)}$ may be much larger than unity and even though the Schottky Conjecture is clearly inappli-
cable, there is need to model such compound structures in terms of the primitive structures, at least in an approximate way. In either case, it is necessary to go beyond the Schottky conjecture in order to determine the AFEF of a compound structure in terms of the primitive AFEF values with some degree of accuracy. The paper is devoted to this endeavour and while no proof is provided, plausibility arguments for a Corrected Schottky Conjecture (CSC) is given along with numerical verification that help us in establishing the usefulness of the CSC for practical compound structures.

Section II deals with the Corrected Schottky Conjecture that may be applied to compound shapes made up of two primitive structures such as hemiellipsoids, paraboloids or a hemiellipsoid on a cylindrical post (HECP). Fig. 1 shows 6 compound structures of which the first 5 [(a) to (e)] are 2-primitive structures. The paper is devoted to this endeavour and while no proof is provided, plausibility arguments for a Corrected Schottky Conjecture (CSC) is given along with numerical verification that help us in establishing the usefulness of the CSC for practical compound structures.

II. THE CORRECTED SCHOTTKY CONJECTURE

In order to appreciate the need for correction terms to the Schottky Conjecture, we shall consider compound shapes made up of two primitive structures such as hemiellipsoids, paraboloids or a hemiellipsoid on a cylindrical post (HECP). Fig. 1 shows 6 compound structures of which the first 5 [(a) to (e)] are 2-primitive structures.

![FIG. 1. A 2-dimensional schematic of 6 axially symmetric compound structures considered here. The five 2-primitive compound structures are (a) an ellipsoid on ellipsoid (b) a paraboloid on ellipsoid (c) a hemiellipsoid-on-cylindrical-post (HECP) on ellipsoid (d) a paraboloid on paraboloid (e) a hemisphere-on-cylindrical post (HCP) on paraboloid, while (f) is a 3-primitive structure consisting of an HECP on a paraboloid which is mounted on an ellipsoid. The top-most primitive structure in each case is referred to as the crown.]

![FIG. 2. The error, as a defined in Eq. (1), as a function of $h_2/R_a^{(1)}$ for 4 compound shapes, each having 2 primitives as shown in (a)-(d) of Fig. 1. The error in the Schottky Conjecture grows as $h_2/R_a^{(1)}$ increases, and is roughly the same for all shapes.]

Fig. 2 shows the relative error in AFEF value of the compound structure (denoted by $\gamma_a^{(C)}$) defined as

$$\text{Error} = \frac{\gamma_a^{(C)} - \gamma_a^{(1)}\gamma_a^{(2)}}{\gamma_a^{(C)}} \times 100 \quad (1)$$

for 4 different combinations of primitives [(a) to (d) of Fig. 1]. In each case the apex radius of curvature of the base, $R_a^{(1)} = 1\mu m$ while the apex radius of the crown is $R_a^{(2)} = 5\mu m$. The first is a hemiellipsoid on top of another (larger) hemiellipsoid, the second is a paraboloid on top of a hemiellipsoid, the third an HECP structure on top of a hemiellipsoid and finally, we consider a paraboloid on top of another paraboloid. In the first 3 cases, the total height of the compound structure is 3$\mu m$ while the total height of the last case is 6$\mu m$. The quantities $\gamma_a^{(C)}$, $\gamma_a^{(1)}$ and $\gamma_a^{(2)}$ have been evaluated using COMSOL. In all cases, the error grows with $h_2/R_a^{(1)}$. It is around 12% when $h_2/R_a^{(1)} = 0.1$, and is as high as 50% when $h_2/R_a^{(1)} = 0.5$. Thus, the Schottky Conjecture seems to holds good when $h_2/R_a^{(1)}$ is very small but the error grows as the protrusion on top of the first structure increases in height compared to the apex radius of curvature $R_a^{(1)}$. Note that despite the variation in the composition of the compound structures, the error is
roughly the same for all shapes. It is thus obvious that a correction to the Schottky Conjecture must principally be a function of $h_2/R_a^{(1)}$.

Clearly, the compounding process wherein a smaller structure (crown) sits on top of a larger base, leads to an amplification of the local field. The equipotential curves that existed close to the apex of the primitive-base (in the absence of the crown), now have to cling to the crown and get further compressed due to the enhancing effect of the smaller structure. When the height of the crown ($h$) is vanishingly small, the local field that existed at the apex of the primitive-base ($E_0\gamma_a^{(1)}$) gets amplified to $E_0\gamma_a^{(1)}\gamma_a^{(2)}$ at the apex of the crown. However, as the height of the crown gets larger, it is not obvious whether the field that get amplified by the factor $\gamma_a^{(2)}$ is the one at the apex of the primitive-base or one that depends on the height of the crown.

To test this, consider the 2-primitive compound structure consisting of a hemiellipsoid as the base ($R_a^{(1)} = 1000\text{nm}$, $h_1 = 2900\text{nm}$, $\gamma_a^{(1)} = 4.84$) and a hemiellipsoid on a cylindrical post (HECP) as the crown ($R_a^{(2)} = 10\text{nm}$). The height of the HECP ($h_2$) is varied from 200nm to 7100nm. Thus $\gamma_a^{(2)}$ varies as does the AFEF of the compound structure. We are interested in the quantity $\gamma_a^{(C)}/\gamma_a^{(2)}$ where $\gamma_a^{(C)}$ corresponds to the apex field enhancement factor of the compound structure while $\gamma_a^{(2)}$ is the AFEF of the HECP (i.e. the crown). In the limit $h_2/R_a^{(1)} \rightarrow 0$, $\gamma_a^{(C)}/\gamma_a^{(2)}$ should approach the AFEF of the base (i.e. $\gamma_a^{(1)} = 4.84$). For all other values it should give an effective enhancement factor corresponding to the field that get amplified by the crown.

Fig. 3 shows the values of $\gamma_a^{(C)}/\gamma_a^{(2)}$ at a few values of $h_2/R_a^{(1)}$ (denoted by circles). As mentioned, in the limit $h_2 \rightarrow 0$, $\gamma_a^{(C)}/\gamma_a^{(2)} \rightarrow \gamma_a^{(1)}$. Indeed Fig. 3 shows such a trend while as $h_2$ becomes large, $\gamma_a^{(C)}/\gamma_a^{(2)} \rightarrow 1$. Thus, the field that gets amplified by the factor $\gamma_a^{(2)}$ is smaller than the field at the apex of the primitive-base for non-zero values of $h_2$. Note that the field at a height $h_2$ above the apex of the primitive base is close to $E_0$ when $h_2 \lesssim 2R_a^{(1)}$. Thus, $E_0\gamma_a^{(C)}/\gamma_a^{(2)}$ is smaller than the field at the apex of the primitive-base but larger than the field at a height $h_2$ above the apex of the primitive-base. As seen in Fig. 3 $1 \leq \gamma_a^{(C)}/\gamma_a^{(2)} \leq \gamma_a^{(1)}$.

Fig. 3 also shows the averaged quantity (denoted by squares)

$$\langle \gamma_a^{(1)} \rangle = \frac{1}{h^2} \int_{h_1}^{h_1+h_2} E_z(z)dz = \frac{\langle E_z(z) \rangle}{E_0}$$

(2)

where $h_1$ is the height of the primitive-base and $E_z(z)$ the field along the axis, calculated here using COMSOL. Clearly $\langle \gamma_a^{(1)} \rangle$ follows $\gamma_a^{(C)}/\gamma_a^{(2)}$ closely over a range of $h_2/R_a^{(1)}$. Thus, it is the average field above the base that gets amplified by the crown by a factor $\gamma_a^{(2)}$. This leads us to the Corrected Schottky Conjecture (CSC):

$$\gamma_a^{(C)} \sim (\gamma_a^{(1)})\gamma_a^{(2)}$$

(3)

for a 2-primitive system, while for an $N$ primitive compound structure

$$\gamma_a^{(C)} \sim \gamma_a^{(N)} \Pi_{i=1}^{N-1} \gamma_a^{(i)}$$

(4)

where the averaging at the $i^{th}$ primitive stage is over the height $h_{i+1}$ of the next stage. Eq. (4) is a useful approximation when successive stages are not limited by the smallness criterion. Rather $h_{i+1}/R_a^{(i)}$ may in fact be larger than 1 as illustrated in Fig. 3. The CSC as in Eq. (4) has been similarly tested for other compound structures. As another example, the base is considered to be a paraboloid of radius of curvature $R_a^{(1)} = 1\mu\text{m}$ and height $h_1 = 5.525\mu\text{m}$ while the crown is a hemisphere on a cylindrical post (HCP) with $R_a^{(2)} = 5\text{nm}$ and total height $h_2 = 475\text{nm}$ (see schematic (e) of Fig. 1). For this system, the average error in CSC prediction is about 2% while the error in Schottky Conjecture is about 45%.

![FIG. 3. The values of $\gamma_a^{(C)}/\gamma_a^{(2)}$ (solid circles) is plotted alongside $\langle \gamma_a^{(1)} \rangle$ (solid squares) defined by Eq. (2).](image-url)

Apart from special primitive-bases such as the hemiellipsoid, the exact axial electrostatic field is in general unknown and hence $\langle \gamma_a^{(1)} \rangle$ can only be evaluated numerically, for instance using COMSOL. However, when $h_{i+1}$ is smaller than $h_i$, it is possible to express the electrostatic field approximately using the nonlinear line charge model [20] so that a simple useful approximation for $\gamma_a^{(C)}$ can be arrived at.

The field $E_z$, above the apex of a generic axially symmetric emitter of apex radius of curvature $R_a^{(1)}$ and height $h_1$, can be approximately expressed using the nonlinear line charge model as (see Eq. (38) in [20] with $\rho = 0$).
\[ E_z \simeq \frac{f(L)}{4\pi\epsilon_0} \frac{2zL}{z^2 - L^2} (1 - C) \]  \quad (5)

where \( z \) is measured from the cathode plane, \( L \) represents the extent of the line charge with \( L^2 \simeq h_1 (R_a^{(1)} - R_a^{(1)}) \), \( f(L) \) is related to the line charge density and \( C \) is a correction term that is unknown \textit{a priori} and arises from the nonlinearity in line charge distribution. It (i.e. \( C \)) is zero for a hemiellipsoid (linear line charge) and in general varies with the shape of the emitter. Importantly, for sharp emitters \( (h_1/R_a^{(1)} >> 1) \) the correction is in general small. Even though the primitive-bases considered here are not necessarily sharp, we shall neglect \( C \) hereafter as a reasonable approximation. Note also that \( 2zL/(z^2 - L^2) \) in Eq. \((5)\) is the leading term and there exists a logarithmic correction \( 20) (\propto \ln((z + L)/(z - L))) \) which cannot be neglected for larger \( z \). For sharp emitters where \( L \simeq h_1 \), the logarithmic contribution is less than half for \( z = 1.2h_1 \) so that Eq. \((5)\) can be considered to be reasonably valid for \( z < 1.2h_1 \).

Writing \( z = h_1 + \Delta \), and using \( 40\), the above equation can be expressed as

\[ \frac{f(L)}{4\pi\epsilon_0} \frac{2h_1 L}{h_1^2 - \Delta^2} \simeq \gamma_a^{(1)} E_0 \]  \quad (6)

the electric field averaged over the height of the crown is

\[ E_z(\Delta) \simeq E_0 \gamma_a^{(1)} (1 - C) \frac{h_1 + \Delta}{h_1} \frac{1}{1 + \frac{2h_1(\Delta + \Delta^2)}{h_1 R_a^{(1)}}} \]  \quad (7)

For small protrusions \( (h_2/h_1 < 0.2) \) from the primitive-base, \( \Delta/R_a^{(1)} \) as well as \( \Delta/h_1 \) are small. Thus, the field along the axis for \( \Delta < h_1 \) is

\[ E_z(\Delta) \simeq E_0 \gamma_a^{(1)} \frac{1}{1 + \frac{2\Delta}{R_a^{(1)}}} \]  \quad (8)

Eq. \((8)\) serves as a reasonable approximation for calculating \( \langle \gamma_a^{(1)} \rangle \) even though, the neglect of \( C \) and the logarithmic term are sources of minor errors.

The electric field averaged over the height of the crown is

\[ \langle E_z \rangle \simeq E_0 \gamma_a^{(1)} \frac{R_a^{(1)}}{2h_2} \ln \left(1 + \frac{2h_2}{R_a^{(1)}}\right) \]  \quad (9)

where averaging has been performed from the apex \( (\Delta = 0) \) to a height \( h_2 \) above the apex. Thus,

\[ \gamma_a^{(C)} \simeq \gamma_a^{(2)} \gamma_a^{(1)} \simeq \gamma_a^{(2)} \gamma_a^{(1)} \frac{R_a^{(1)}}{2h_2} \ln \left(1 + \frac{2h_2}{R_a^{(1)}}\right) \]  \quad (10)

Eq. \((10)\) thus provides a useful approximation for the apex field enhancement factor of 2-primitive compound structures when \( h_2 < 0.2h_1 \). It can be generalized for \( N \)-primitive compound structures and can be expressed as

\[ \gamma_a^{(C)} \simeq \gamma_N \Pi_{n=1}^{N-1} \gamma_a^{(n)} U_n = \gamma_a^{CSC} \]  \quad (11)

where

\[ U_n = \frac{R_a^{(n)}}{2h_{n+1}} \ln \left(1 + \frac{2h_{n+1}}{R_a^{(n)}}\right) \]  \quad (12)

We refer to Eq. \((11)\) as the Corrected Schottky Conjecture for small protrusions. When \( \frac{2h_{n+1}}{R_a^{(n)}} << 1 \), a few terms in the expansion of the logarithm

\[ U_n = \left[1 - \sum_{k=1}^{\infty} (-1)^{k-1} \frac{2^k}{k+1} \left(\frac{h_{n+1}}{R_a^{(n)}}\right)^k\right]. \]  \quad (13)

provides a useful approximation for \( U_n \): Typically, for \( h_{n+1}/R_a^{(n)} < 0.05 \), less than 5 terms suffice.

III. NUMERICAL VERIFICATION

The Corrected Schottky Conjecture takes into account the electrostatic field averaged over the height of successive protrusions. It thus corrects the over-estimation of the apex field enhancement factor of the compound structure. To see how effective this prescription is, we consider the 2-primitive compound structures considered earlier.

![FIG. 4. The relative error, as defined in Eq. (14), as a function of \( h_2/R_a^{(1)} \) for the 4 compound shapes considered in Fig. 2](image-url)
where the expression in Eq. (11) is used for $\gamma_a^{(CSC)}$ while $\gamma_a^{(1)}$, $\gamma_a^{(2)}$, and $\gamma_a^{(3)}$ have been obtained using COMSOL. A comparison of Figs. 2 and 4 shows the vast improvement in prediction of the Corrected Schottky Conjecture (CSC) especially at higher values of $h_2/R_a^{(1)}$. Thus, Eq. (11) can serve as a simple useful formula to estimate the apex field enhancement factor of compound structures in terms of the primitive components.

IV. DISCUSSIONS AND CONCLUSIONS

In the previous sections, we have proposed and verified a Corrected Schottky Conjecture (CSC) which may be expressed as: the apex field enhancement factor (AFEF) of a compound structure consisting of $N$ primitive structures is approximately the product of the crown AFEF and the product of the average AFEF of all the $N - 1$ primitive-bases, the average being over the height of the structure on top of each primitive-base. If the height of the structure on top of each primitive base is much smaller than the height of the primitive base, the CSC may be expressed using a simple approximate formula given by Eq. (11).

The Corrected Schottky Conjecture was found to be a useful approximation for determining the apex field enhancement factor of compound structures under much relaxed conditions. The effectiveness of Eq. (11) for an $N$-primitive compound structure may be limited by the approximate additive law of relative errors that is expected to hold as indicated by the results of the 3-primitive example together with Figs. 2 and 4 for the original and corrected Schottky Conjecture. Thus, if $N$ is large, the ratios $h_{i+1}/R_a^{(i)}$ must be small enough for the CSC of Eq. (11) to have useful predictive capability. An aspect that has not been discussed so far involves primitive structures with (finite sized) flat tops. Our numerical studies show that the CSC in its generality (in terms of average enhancement factors) applies here as well within reasonable errors.

Finally, the Schottky Conjecture has sometimes been invoked to justify large values of the field enhancement factor as derived from experimental Fowler-Nordheim (FN) plots in field emission studies. A couple of cautionary notes seem necessary. First, the use of the elementary field emission equation, which uses the exact triangular barrier tunneling potential results in unphysically high values of the enhancement factor to compensate for the larger barrier height. The actual enhancement factor required to explain an experimental $I - V$ plot is always much lower when using a variant of the Murphy-Good expression for the current density which uses the Schottky-Nordheim potential that includes the image-charge contribution. For smooth curved emitter tips, the curvature corrected expression for the current has been found to give results consistent with the physical measurements and may therefore be used directly to determine the value of the enhancement factor.

The second cautionary note follows from Fig. 3. Note that $\gamma_a^{(C)}/\gamma_a^{(2)} \rightarrow 1$ as $h_2/R_a^{(1)}$ becomes large. Thus a tall structure (such as a nanotube or nanowire) on top of a curved base will not enjoy the multiplicative effect of the base as the field $E_z(z) \rightarrow E_0$ for $z$ large so that the average enhancement factor is close to unity. The Schottky Conjecture thus cannot be used to justify the values of enhancement factors of compound structure having a tall crown. This is of particular importance in multiscale modelling of field emitter.
a separate analysis that seems challenging and is beyond the scope of the present manuscript.

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