Effect of electrical conduction on the electron emission properties of diamond needles

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Keywords: diamond, field emission, voltage loss, Fowler–Nordheim, Poole–Frenkel

Abstract

Single crystal diamond needles are promising structures as point electron sources. However, the low electrical conductivity of diamond limits their application as high brightness electron sources. Here we study experimentally and numerically the field emission behavior of single crystal diamond needles, in order to better explain the link between the low electrical conduction, the non-homogeneous field distribution in the needle, the evolution of the field enhancement factor and the saturation of the Fowler–Nordheim plot. Field emission current and voltage loss were measured as a function of the applied voltage. Numerical modelling was used to solve conduction, emission and Laplace equations taking into account the real geometry of the field emitter and its environment. The combination of experimental and numerical results shows that the conduction behavior and the field enhancement factor depend on the diamond geometry. Moreover, the Fowler–Nordheim plot saturation is shown to be affected by the electrostatic environment which can limit the range of voltage losses that can appear along the diamond needle and hence limit the field emission current. At the same time, the increase of the emission current at high field, which is sometimes argued to be caused by the breakdown of the field emitter, is here presented as a simple consequence of the conduction properties of the field emitter as it was already shown for silicon field emitters.

1. Introduction

Stimulated by promising applications such as electron guns, flat panel displays, or ultrafast electron microscopy, a considerable research effort has been made during the past years on field emission electron sources. Wide band-gap materials, and in particular diamond, have been identified as suitable for field emission purposes due to their low or even negative [1] electron affinities, as well as their thermal, chemical, and mechanical stability ([2–4]). Although progress has been made in technological realization of microtip diamond field emission cathode, such as polycrystalline diamond emitters [5] or single-crystal diamond needles [6, 7], the low electrical conductivity of intrinsic wide band gap diamond limits the electron emission as revealed by their Fowler Nordheim's law. Because of diamond’s high resistivity, a voltage loss can occur along the needle when the current flowing through it is sufficiently large. Moreover, this current–induced voltage loss (or drop) along the emitter is directly and inexorably linked to a reduction in the field enhancement factor, implying a lower surface field at the emitter’s apex and hence an emission current lower than predicted by Fowler Nordheim’s law. This link with the field enhancement factor was first shown, experimentally and numerically, on carbon nanotube emitters by Minoux et al [9] and, recently, analytically demonstrated by Forbes [10], on the simple cylindrical-post field-emitter geometry. However, diamond needles have a conical geometry, which can strongly impact their electrical conduction behavior, as recently discussed by authors [11], compared to that of a nanowire shaped emitter, changing the voltage-loss-current dependence and hence, the field.
This work provides a coupled numerical and experimental study of the field emission properties of a single-crystal diamond needle glued on a tungsten (W) microtip. Experimentally we measure the electron emission current and the induced voltage loss, as a function of the applied voltage. We compare these results with a numerical model taking into account the geometry of the sample as measured by scanning electron microscopy (SEM), as well as its environment. We use this information to calculate the non-homogeneous field distribution in diamond, at the microscopic scale, as well as the value of the electric field in the emission region. We highlight two different emission regimes depending on the emission current. At low current, the emission is limited by the emission process, and at high current it is limited by the conduction process, the latter regime producing emission curves that are characteristic of the conduction mechanism. We also find that our results are compatible with conduction through the bulk of diamond as opposed to its surface. Regarding the link between the voltage loss and the field enhancement factor, we also prove that in the case of emitters that have both a varying cross section, and a non-linear resistivity, the evolution of the field enhancement factor deviates for the linear behavior reported by Minoux et al [9] and Forbes [10]. And last, when the emission is conduction limited, the only way to maximize the emission current is to maximize the emitter’s internal electric field. We find that this can be optimized by selecting the geometry of the emitter and its surroundings, in our case for example, the geometry of the support needle.

The article is structured as follows: we first describe the experimental results regarding emission currents and energy of the emitted electrons. We then show how the conduction characteristics of diamond were calculated and used to extract information from experimental data. We then show how the obtained potential distribution is used to calculate the electrostatic environment of the needle, and we discuss its implications on the sample geometry on the field enhancement factor. In the last section we calculate the needle’s emission current and compare the results with the experimental data.

2. Experimental and numerical results and discussions

2.1. Current and voltage loss characterization

Four diamond needles were glued on tungsten support tips and were each placed in a field emission apparatus equipped with an electron spectrometer (see section 4—samples and methods). The measured currents ($I$) are represented for each tip as a function of the applied voltage $V_0$, in Fowler-Nordheim coordinates in figure 1. All four diamond needles show non-linear behavior, with a negative curvature for needle (2), and a positive curvature for needles (1), (3), and (4). This is contrary to what would be expected for a metal for example. Here, this deviation from a straight line is caused by the resistivity of diamond. It causes a voltage loss along the diamond needle and thus changes in the field enhancement factor $\beta$.

The current-induced voltage loss $\Delta V$ as a function of the measured current is reported for the four samples in figure 2. We can note that the variation of the voltage loss is non-linear as a function of the enhancement factor. It simply follows that field-emission properties will then be strongly affected by the changes in the field emitter geometry and the surrounding environment.

Figure 1. Fowler–Nordheim plots of the field emission characteristics for diamond needles (1), (2), (3) and (4).
current, which means that the resistivity of diamond is non-constant. It can also be noted that the values of the currents emitted by the different needles differ by orders of magnitude for similar values of voltage losses.

2.2. Conduction through diamond

In fact, in diamond, charges flow according to the Poole Frenkel mechanism [12, 13]. Following this mechanism, a large number of electrons are trapped in states near the conduction band and can be freed in the presence of an electric field and contribute to the current. The dependence between the current $I_C$ going through an object and the voltage loss $\Delta V$ along the considered axis is generally given by equation (1) [8, 14]:

$$I_C = A \Delta V \exp \left( B \sqrt{\Delta V} \right),$$

(1)

where $A$ and $B$ are parameters that depend on the object’s properties as well as geometry. This expression, however, is valid only when the electric field is homogenous inside the emitter, which means that it has to have a constant cross section as it is the case for a thin films or nanowires. In our case, however, diamond needles have varying cross sections and should exhibit an inhomogeneous electric field. According to equation (1), plotting $I(\Delta V)$ characteristics in the so-called Poole–Frenkel coordinates should yield a straight line. Our experimental data, however, gives a curve with a positive curvature (figure 3), illustrating the fact that, indeed, equation (1) cannot be used in this application. Moreover, in the case of field emission from diamond needles, it was found that at low currents the conduction behavior was best described as a Poole Frenkel (PF) conduction mechanism in parallel with ohmic conduction, which does result in a positive curvature of Poole Frenkel plots [11]. Thus, we used the following expression, which depends only on the local geometry and intrinsic material properties and also includes a term that accounts for the ohmic current assumed in parallel with PF conduction:

$$I_C = S_C(x) \cdot \left( j_{PF}(x) + j_{\Omega}(x) \right) = S_C(x) \cdot \left( A' E_C(x) \exp \left( B' \sqrt{E_C(x)} \right) + \frac{E_C(x)}{\rho_{\Omega}} \right),$$

(2)

where $I_C$ is equal to the field emitted current (indicated as $I$ in figures 1 and 3), $x$ is the position along the needle’s axis, $j_{PF}$ and $j_{\Omega}$ are the current densities associated to ohmic and Poole Frenkel conduction, $A'$ is a parameter intrinsic to the material that depends, among other things, on the local density of states, $E_C$ is the electric field inside the needle, $\rho_{\Omega}$ is the ohmic resistivity of diamond and $S_C$ is the needle’s local cross section. By using the needle’s cross section, we assume that conduction occurs through the bulk of the diamond needle, as opposed to its surface. Conduction through the surface, however, cannot be ruled out and will be discussed later on. The last parameter of equation (2), $B'$, is given by:

$$B' = \frac{1}{kT} \left( \frac{e^3}{\pi \varepsilon \varepsilon_0} \right)^{1/2},$$

(3)

where, $e$ is the elementary charge, $\varepsilon_0$ and $\varepsilon$ are the absolute and relative permittivity of diamond respectively. For the case of sample 4, which geometry is well known, equation (2) was inversed numerically in order to obtain $E_C(x, I_C)$, which, when integrated from 0 to $x$ gives the voltage distribution along the
needle \( V(x, I_C) \). This distribution varies in a complex way depending on the sample geometry and on the emission current, and was already described elsewhere \[11\].

From this function, values of \( \Delta V \) as a function of applied voltage \( V_0 \) were calculated for comparison with the experiment. \( A' \) and \( \rho_\Omega \) were adjusted so as to obtain the best fit of the experimental data (figure 3).

A value of 5.7 was used for \( \varepsilon \) which is commonly accepted for diamond \[15\]. The values of \( A' \) and \( \rho_\Omega \) that gave the best fit are \( A' = 2.678(86) \times 10^{-13} \) Sm\(^{-1}\) and \( \rho_\Omega = 7.41(13) \times 10^8 \) \( \Omega \) m. We can note that the value of \( \rho_\Omega \) lies within the wide range what is commonly observed for diamond (from \( 10^5 \) to \( 10^9 \) \( \Omega \) m\[16\]), which means that it is at least physically realistic. For comparison, the use of equation (1), describing the Poole Frenkel conduction in a thin film or a nanowire, yields a linear function (here with \( A = 4.54 \times 10^{-19} \) S and \( B = 5.31 \times 10^{-2} \) V\(^{-0.5}\)) that poorly fits the experimental data.

We would like to note that the experimental data was fitted using the bulk value of the relative permittivity of diamond. Therefore our results are compatible with a conduction in the bulk of the diamond as opposed to its surface.

### 2.3. Electrostatic environment and field enhancement factor

Now, in order to calculate the emission current, the potential distribution along the needle’s surface that we have obtained can be used to calculate the electric field distribution around the needle, and more importantly at its apex.

In order to do so, the calculated potential function \( V(x, I_C) \) is injected in the model of the analysis chamber. As an initial condition, the voltage \( V_0 \) is applied to all the needle as well as the sample holder plane, and the current flowing through diamond, \( I_C \), is set to zero, which means that the voltage loss is initially equal to 0. Then the corresponding surface field \( E_E \) at the needle’s apex is calculated by solving Laplace’s equation using the finite element method.

The emission current resulting from this field is then calculated using the equation for Fowler Nordheim tunneling:

\[
I_E = S_E a \Phi^{-1} E_E^2 \exp \left( -v \left( f \right) b \Phi^{3/2} / E_E \right),
\]

where \( a \) and \( b \) are constants equal to and 1.541 \( \times 10^6 \) A \( \text{eV}^{-2} \) and 6.831 \( \text{eV}^{-3/2} \) \( \text{V} \text{nm}^{-1} \) respectively \[17\], \( S_E \) is the surface of the emission region, that was set to 4.9 \( \text{nm}^2 \) based on a measurement performed on a similar diamond sample, \( \varphi \) is the workfunction of diamond which was set to 5 eV \[18\] and \( v(f) \) is given by \[19\]:

\[
v \left( f \right) \approx 1 - f + (1/6) f \ln \left( f \right),
\]

where \( f \) is given by:

\[
f = \left( \frac{e^3}{4\pi\varepsilon_0} \right) \frac{E_E}{\Phi^2}.
\]

An emission current \( I_E \) is found, that is initially different from the conduction current \( I_C \). This difference has no physical reality but is used here only as initial conditions. \( I_E \) is thus modified by an increment and a new value of \( I_C \) is calculated. Using the method of dichotomy \( I_E \) converges towards a value so that \( I_E \) is
equal to $I_C$, as it should be in reality, to an error of 0.1%. This can typically be achieved in about 15 to 20 iterations. These numerical calculations are then repeated for different values of the applied voltage $V_0$.

The obtained surface field can be used to calculate the field enhancement factor $\beta$, defined as:

$$E_k = \frac{\beta V_0}{R}, \quad (7)$$

where $R = 14$ nm is the apex radius of the field emitter, and which depends on the applied voltage $V_0$.

Minoux et al [9] and Forbes [10] had found that beta should decrease linearly with the relative voltage loss. The voltage loss being relative to the applied electric field, in their case, or relative to the applied voltage. The evolution of $\beta$, normalized to $\beta_0 = 0.146$, which is obtained in the case of zero voltage loss, is represented in figure 4 for our conical geometry. Its trend is clearly non-linear. This is likely due to the complex evolution of the potential along the diamond needle, that evolves non-linearly with the total voltage loss. This non-linear evolution is due to the presence of the non-linear Poole Frenkel conduction mechanism together with the fact that the needle has a varying cross section. For comparison, the emission was also simulated, for the same geometry, but retaining only the ohmic contribution, or for a nanowire geometry, of 28 nm diameter, and keeping, this time, both the ohmic and Poole Frenkel conduction mechanisms. In both cases $\beta / \beta_0$ changes linearly with $\Delta V / V_0$ (figure 4).

2.4. Emission current

The emitted current was also calculated and reported in Fowler Nordheim coordinates in figure 5, where it is compared to experimental data.

Although the general trend of the experimental data is well reproduced, there is a large discrepancy between the simulated and experimental data, as shown by the inset in figure 5. Various hypotheses can be used to explain this difference and each will be discussed in the following. We will explore different possible errors regarding the geometry we have used and the conduction mechanisms we have assumed to take place in diamond. The first hypothesis that might explain the observed discrepancy is that, some fraction of the diamond needle could have a very high conductivity, essentially causing short-cuts on fractions of the diamond needle. Indeed, it was already observed that some diamond needles could become highly conductive. This was observed after accidental exposure to the Ga$^+$ ion beam during sample preparation, but also sometimes on fresh diamond needles. It is possible that a fraction of the surface could be covered with a layer of amorphous carbon, as already observed in the literature [20], possibly remaining after the sample preparation, and that would act like an electric short cut. This would locally cancel part of the voltage drop in diamond. In order to test this hypothesis, the top 10% of the diamond needle were made perfectly conductive in the simulation to be compared to the experimental data. This value of 10% was chosen because it gave a result that was still within the range of the experimental data as shown later on.

Another hypothesis could be that conduction occurs only through the surface of diamond, as suggested elsewhere [2] which would induce a different profile of current density and hence, a different electric field along the needle’s axis. In order to test this hypothesis, the current flow was constrained to a layer of 1 nm
Figure 5. Fowler–Nordheim plot of the experimental results obtained for diamond needle (4) (black dots), simulated results (blue solid line) and theoretical emission limited current (green dashed line) and conduction limited current (red dashed line). The inset shows the simulation results with the top 10% of the diamond needle being perfectly conducting, with conduction considered to happen only along the surface of diamond and with the diamond needle located 4 mm away from the grounded grid instead of 5 mm.

on the needle’s surface, which means essentially that conduction occurs on the surface only. The last hypothesis is that the distance between the needle’s apex and the first grid is inaccurate. To test this hypothesis, the simulation was performed with the needle located 1 mm closer to the grid. The results of these simulations are plotted in the inset of figure 5. This value of 4 mm was chosen because it was the value that best fitted the experimental data that was still within the bounds of the uncertainty in the position of the needle. These modifications in the simulation parameters cause a shift in the simulated curve but do not improve the fit quality significantly. Another hypothesis could be that the increase in the emission observed experimentally could be partly due to the onset of breakdown through impact ionization. In bulk diamond, breakdown should happen at a field of $10 \text{ MV cm}^{-1}$ [21], whereas in our case the highest field calculated in diamond, at an applied voltage of 2000 V, is $1 \text{ MV cm}^{-1}$. While it is possible that breakdown starts at such a low field because of the presence of defects, we still believe it is unlikely given the high quality of the fit of the conduction data in figure 3, that was obtained using only the approximation of ohmic and Poole Frenkel conduction. It is possible, however, that the observed discrepancy is caused by inaccuracies in the simulation geometry, namely the presence of objects in the chamber that were not considered because of symmetry constraints and/or inaccuracies in the morphology of the diamond and metallic support needle entered in the simulation, that were estimated from two-dimensional images.

Nevertheless, the trend and curvature of the experimental data is well reproduced by the simulations. In figure 5, emission was also simulated for currents and voltages well beyond those that are accessible experimentally using our setup. Naturally, these results should not be used as a trustworthy extrapolation of the experimental data, but only as a trend that shows, qualitatively, what features of the Fowler Nordheim plot should be expected given the approximations of the present model.

Nevertheless, different emission regimes can be observed depending on the emitted current. In the low current regime, on the right-hand side of the plot, the emission exhibits a perfectly linear behavior. Then in the high current regime, the emission almost plateaus and then rises sharply at voltages higher than 1500 V. These regimes can be explained in the following way: at very low current the voltage drop along the diamond needle is negligible, and the field enhancement factor $\beta$ in equation (7) remains constant when $V_0$ is increased. Using equation (7) to replace $E_k$ in equation (4) gives

$$I_e = S_e a \Phi^{-1} \left( \frac{V_0 \beta}{R} \right)^2 \exp \left( -v \left( f \right) b \Phi^{3/2} / \left( \frac{V_0 \beta}{R} \right) \right).$$

Equation (8) is plotted in figure 5 using these values (green curve) and highlights the fact that the simulated emission does follow a purely Fowler–Nordheim trend, as for a metal, and then deviates from this line when $V_0$ exceeds 200 V. Thus, in this first regime, the emission current is entirely limited by the field emission process and is unaffected by the conduction processes.
Then as the voltage (and hence the current) increases further, the relative voltage loss becomes significant. This relative voltage loss, however, cannot increase indefinitely. Indeed, even in the absence of diamond, the metallic support needle already generates an electric potential in its surroundings. One can assume that in the presence of diamond, the apex potential will never decrease below the potential generated by the support needle at the same position, as this would mean that the surface electric field is almost cancelled or negative and would prevent field emission. Therefore, as a first approximation, this potential can be considered as the minimum attainable voltage at the diamond’s apex. The potential generated by the support needle alone, was calculated using the same finite element model and is represented in figure 6 along the direction of the diamond needle.

In this second regime, we assume that at high current, the voltage drop completely saturates and is always at the maximum value:

$$\Delta V_{\text{max}} = \alpha V_0,$$

where $\alpha$ is a constant. In the case of our geometry, the calculated value for $\alpha$ is 0.42. This value, of course, should depend on the geometry of the chamber as well as that of the support needle. Assuming that at high voltage $\Delta V = \Delta V_{\text{max}}$, and that Poole Frenkel conduction is the dominant mechanism, as it should be for high currents [11] and reducing Poole Frenkel conduction to equation (1) for the sake of simplification, and combining equations (1) and (9) gives:

$$I_C = A\alpha V_0 \exp \left( B\sqrt{\alpha V_0} \right).$$

This function is plotted in figure 5, as a red dashed line. Its shape is very similar to that of the simulated data for applied voltages above 300 V, including the positive curvature at very high voltage, and a sharp emission increase above 1500 V. It is however located at an offset from the simulated data. This is mainly due to the fact that the method used here to determine the voltage drop gives an overestimated value, because not only the support needle affects the electrical potential in the emission region but so does the shank of the diamond needle, reducing the value of the maximum attainable voltage drop. Nevertheless, we show that at high voltage, the emission saturates and enters a regime where the current is mainly controlled by the conduction process in diamond, and not so much by the emission process itself. In this regime, the positive curvature of the emission curve can be explained solely by the fact that the current is limited by the Poole–Frenkel conduction along the diamond needle, and without necessarily relying on impact ionization as it was also reported for silicon field emitters [22, 23]. Contrary to these studies, however, we demonstrate the morphology of this saturation curve taking into account a complex emitter morphology. Also, in this regime, the voltage loss, and thus the emission current, is constrained by the electrostatic environment of the diamond emitter. It follows that the geometry of the diamond needle should have an effect on the emission, but so should the geometry of the chamber and especially the metallic support needle. These effects contribute to explain the variety of behaviors that have been observed in the Fowler Nordheim plot for the different samples in figure 1, with positive or negative curvatures of the emission characteristics. The
morphology of both the diamond needles and tungsten support needles having little repeatability, it most probably causes different diamond needles to each emit in a different regime. Other phenomena are also likely affecting the value of the emitted current, as shown by the very high current emitted by needle (1) in figures 1 and 2, which is six orders of magnitude higher than that of needle (4) despite similar values of voltage loss. Such a difference in behavior is more likely to be explained by differences in material characteristics, such as a higher concentration of traps in the case of needle (1), resulting in a higher pre-exponential factor $A'$ in equation (2). However, regarding the samples’ geometry, if one wanted to maximize the emitted current, one strategy should be to maximize the electric field in diamond. In order to do so, our results show that the electrostatic impact of the support needle should be reduced to a minimum, so it should have a small cone angle and radius of curvature, and ideally, the diamond needle should be as short as possible. As shown schematically on figure 6 reducing the length of diamond to half of its value decreases the value of the maximum voltage drop by less than a factor of two, which means that a shorter needle results in a higher electric field inside diamond, and thus a higher emission current in the conduction limited emission regime. This supports the idea of using diamond as a thin coating directly deposited on a metallic needle [24] for example.

3. Conclusions

As a conclusion, the numerical calculation performed taking into account the geometry of the diamond needle and the electrostatic environment, have been useful to demonstrate that the conduction behavior of the diamond needle (in term of the $I$–$\Delta V$ plot) is geometry dependent. They also demonstrate that the results are compatible with a conduction through the bulk of diamond although conduction through the surface can also not be ruled out. We also observe that the field enhancement factor has a non-linear behavior as a function of the relative voltage loss. This non-linearity is caused by the sample’s geometry together with the non-linear conduction mechanism in diamond. We determine this behavior for a real, non-nanowire, field emitter morphology for the first time. Regarding diamond’s emission current, we have identified two emission regimes depending on the magnitude of the voltage loss along the diamond needle. At low currents, the voltage loss is negligible and the emission follows a perfect line in Fowler–Nordheim coordinates, and therefore the current is emission limited. At high current, the relative voltage loss approaches its maximum value and the emission characteristics strongly deviate from the linear behavior and instead follow a trend which shape is determined solely by the conduction mechanism, and therefore the current is conduction limited. The occurrence of one regime or the other or a transition between the two should depend not only on the morphology of the diamond needle but also on that of the metallic support needle, which explains the variety of Fowler–Nordheim plots morphologies observed experimentally.

Finally, this work shows that the electrostatic environment of diamond needles (but more generally wide band-gap field emitters) has to be chosen carefully in order to maximize the possible voltage loss, and therefore the electrostatic field, along the emitter. This maximizes the current that can potentially go through the emitter, as well as the conductivity, in the case of a Poole Frenkel conduction, and, hence, the field emitted current and the brightness of these point-emitter electron sources.

4. Samples and methods

The diamond needles were obtained by growing a carbon film by CVD, containing single crystalline diamond needles embedded in an amorphous matrix. The amorphous carbon was then removed by selective oxidation. This method yields pyramid shaped diamond needles with a radius of curvature down to about 10 nm. More details about this fabrication method can be found in [6]. These needles were then dispersed on a substrate and four of them were glued to tungsten needles either under an optical microscope equipped with a micromanipulator, or in a focused ion beam (FIB) apparatus, using a piezoelectric micromanipulator and ion beam induced platinum deposition. The needles that were selected for analysis ranged from 14 to 70 $\mu$m in length. When FIB was used, care was taken to image the diamond needles with the ion beam only within a few micrometers of the region where platinum was deposited, so as to keep the majority of the diamond needle free from implantation damages that could affect its conduction properties.

Before performing electron emission, different procedures were used to condition the needles and evaporate adsorbates from their apex region. Needles (1) and (4) were subjected to a voltage of +2.5 kV while being exposed to a 120 mW laser ($\lambda = 1030$, 300 fs pulse duration, with a spot size of a few micrometers) focused on the needle’s apex for 1 h, and needles (2) and (3) were subjected to positive
voltages above +5 kV followed by cycles of voltages lower than −2 kV until field emission could be observed for voltages above −2 kV, i.e. yielding electrons with energies that are within the range of the spectrometers that were used.

Their electron emission current as well as energy were then characterized. For practical reasons, this was performed using different instruments for each needle: using a retarding field energy analyzer equipped with a microchannel plate detector for electron counting (needle (1), see [8] for more details, and needle (3)), using a hemispherical energy analyzer (needle (2)) (Argus CU—ScientaOmicron) or last, by counting electrons using a channeltron separated from the sample by a flat grid of high transparency (needle (4)). In the first case, the current was measured using a picoammeter placed between the high voltage power supply and the diamond needle, and in the case of needles (2) and (3) the current given herein corresponds to the raw number of detected electrons per unit time. In the last case, needle (4), the current was calculated from the measured electron count rate corrected for the grid’s transparency and detection efficiency (40% detection efficiency in total). This correction factor was calibrated based on the current emitted from a tungsten needle, measured with the picoammeter at high current and extrapolated to low currents using Fowler Nordheim’s law. In this last case, the electrons energy was determined by increasing the channeltron’s potential until no more emission was observed and this cutoff voltage was used for the calculation of the electron energy.

The voltage loss was then calculated using (11):

$$\Delta V = V_0 - \frac{Ee^-}{e} = V_0 - V_{\text{cutoff}}$$  \hspace{1cm} (11)

where $V_0$ is the voltage applied to the needle, $Ee^-$ is the electrons energy, $e$ is the elementary charge and $V_{\text{cutoff}}$ is the cutoff voltage. Similar data were already obtained for diamond by the same authors [3, 8, 11].

The electrostatic environment of the sample was also simulated. In order to do so, the geometry of the sample and experimental setup must be known. For this reason, only needle (4) was simulated because it was the only one for which the complete geometry had been characterized as well as its electrostatic environment and the current was measured most accurately. The morphology of the diamond needle itself was characterized by SEM (figure 7), as well as that of the tungsten support needle (not shown here).

The model of the analysis chamber used for numerical calculation is as follows: the tungsten support needle is 10 mm long and the apex is located 5 mm away from the grounded grid that acts as a counter electrode. It is assumed that the whole simulation geometry has cylindrical symmetry so as to allow a simple two-dimensional calculation (figure 8). The geometry space is meshed using a random adaptative mesh.

The voltage distribution along the diamond needle ($x$ axis) has been simulated taking into account different conduction mechanisms, as presented in detail in the results and discussion section. The corresponding conduction equations were solved numerically using a step size of 70 nm. The surface field $E_s$ at the needle’s apex was calculated by solving Laplace’s equation in the whole geometry using the finite element method.

The effect of band bending in diamond was neglected, however. In fact, as calculated by Tsong [25] for intrinsic silicon and germanium and Arnoldi et al [26] for MgO, a large band-gap material such as diamond, the surface band-banding and the field penetration depth are negligible compared to the band-bending and the field penetration induced by conduction mechanisms in the emission regimes.
Acknowledgments

The authors would like to thank Pr. Obraztsov for providing the samples that were used in this study. This work was supported by the French Agence Nationale de la Recherche (ANR), through the program 'Investissements d'Avenir' (ANR-10-LABX-09-01 and ANR-11-IDEX-0002-02, reference ANR-10-LABX-0037-NEXT, ANR-13-BS04-0007-01), LabEx EMC3, Efesto Project, by the European Union with the European Regional Development Fund (ERDF) and the Regional Council of Normandie.

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