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Electron Transverse Energy Distribution in GaAs Negative Electron Affinity Cathodes: Calculations Compared to Experiments[◊]

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ABSTRACT

The transverse momentum of photoelectrons released from an NEA GaAs cathode is small compared with other thermonic or field emission electron sources. A low photoelectron transverse momentum in vacuum promises highly focused, low-energy beams useful for numerous applications.

A simplified theory for electron emission from GaAs predicts much lower electron transverse momentum than those previously measured experimentally. To address this theory-experiment mismatch, Monte-Carlo based calculations were compared with experimental data. We checked the possibility of there being electron scattering in the Cs,O layer; however, none of the scattering checked (isotropically-distributed, cosine-distributed, and Rutherford scattering) properly fit the experimental results. The assumption of conservation of the parallel component of the crystal momentum k during the emission is mainly believed to be responsible for the calculation-theory disagreement. The best simulation-experiment fit was obtained through a relaxation of the conditions imposed on the transverse momentum inside and outside of the semiconductor when an ideal interface is considered. We obtained the best results by assuming that the effective-mass of the electron inside GaAs is equal to the effective-mass of the electron in vacuum. Two independent experiments confirmed that in both cases, this *same-mass* approximation gives the best fit. The *physical* meaning of this is not clear, but it seems to be related to the amorphous nature of the Cs,O layer. We conclude that the way to get lower electron transverse energy spread cathodes is to study alternative activation methods and new materials with smaller effective electron masses.

INTRODUCTION

Applications of Negative Electron Affinity (NEA) photocathodes are rapidly increasing. In an NEA cathode, the vacuum level at the surface lies below the bulk conduction band minimum. A wide variety of technologies essential for manufacturing microelectronic devices demand small spot-size and low-energy beams. These include microscopy, lithography, Auger spectroscopy, microanalysis, LEED and high-speed time-domain electron beam metrology. NEAs are naturally large (~1 cm^2 or larger) and planar, with uniform emission over their surface. They have a small energy spread (typically less that 100 meV), high brightness (~10^8 A/cm^2-sr [1]), and the possibility of emission from small areas (<1 μm). All these things make NEAs one of the best choices of electron source for the next generation of electron guns.

Beam brightness is mainly determined by the angular distribution of the emitted electrons. Narrow angle electron emission is critical for achieving a high quality electron beam. Pollard reported [2] very narrow angular distributions for electrons from GaAs (100) and (111)B, activated with Cs, using a LEED–AES experimental setup. Pollard observed electron emission in a very narrow cone (~4° half-angle). As far as we know, no subsequent measurement of the angular distribution from GaAs NEA cathode shows such a narrow cone emission [3.4]. Bradley et al. claimed [3] that the experimental setup used by Pollard was not the best choice for making electron angular distribution measurements because of problems with electrostatic fields. The electron transverse energy is the average energy associated with the k-component parallel to the emitting surface. It is currently accepted that the electron transverse energy from the GaAs NEA cathode is almost an order of magnitude higher than that predicted for a simple theory of electron emission from an ideal interface; it is also an order of magnitude higher than Pollard reported in his work.

Because future technological applications demand high-brightness electron sources, knowledge of the mechanisms present during the electron emission to the vacuum is necessary for improving the actual performance of these devices. Our purpose here is to review the current state of the art in order to shed light on the angular emission process from NEAs, and to give some direction as to which areas must be addressed in order to achieve continued improvement.

Section 1 presents a simple model showing predictions for angular distribution from the NEA GaAs cathode. Data shown are the results of a computer simulation of electrons from a GaAs transmission-mode cathode. The cathode used was a standard, high-yield GaAs cathode, such as that used in night vision devices. We compare our calculations with the results of the experiment described in Fig. 1 [5].

Section 2 discusses possible causes of the calculation-experiment mismatch.

Section 3 is a general discussion of the problem, with suggestions for improving the actual performance of the cathodes.

1. CALCULATION COMPARED TO EXPERIMENT

The Monte Carlo simulation begins when the electrons, previously photoexcited and thermalized at the conduction-band minimum, reach the band-bending region. There, they are under the influence of a very high electric field, typically $>1\times10^{6}$ V/cm, and the electrons gain enough kinetic energy to excite phonons in the lattice. The final result is that the initial narrow energy distribution corresponding to thermalized electrons is transformed into a broader energy distribution when the electrons cross the band-bending region. A detailed description of the Monte Carlo simulation can be found in Refs. [6] and [7].

The condition necessary for an electron to escape when it reaches the surface is

$$E_L > VL \tag{1}$$

where E_L is the component of the energy associated with momentum perpendicular to the semiconductor-vacuum interface and VL is the Vacuum Level. If we assume an *ideal semiconductor-vacuum interface,* the total energy and the momentum parallel to the interface must be conserved during the emission. When we impose the conservation laws and equate the crystal transverse momentum $\hbar k$ to transverse momentum in the vacuum, the electron transverse energy in the vacuum, E_{To}, is related to the transverse energy in the semiconductor by the following expression:

$$E_{To} = E_T\,(m^*/m_o) \tag{2}$$

For electrons from the GaAs Γ valley, the value of their transverse energy in vacuum is reduced almost 15 times the value that was inside the semiconductor prior to emission. Because of the conservation of the total energy, the kinetic energy "lost" in the transverse direction is transferred to the longitudinal direction; the relationship between the longitudinal energies inside, E_L, and outside, E_{Lo}, the semi-conductor would then become

$$E_{Lo} = E_L + (1-m^*/m_o)\,E_T \tag{3}$$

Figure 2 illustrates this effect, which is like a refraction suffered by the electrons as they are crossing the interface between two different materials, each with a different electron effective-mass. The magnitude of this effect is directly related to the difference in the electron effective-masses inside the semiconductor and in the vacuum; we therefore call it the *mass effect*.

Figure 3 shows the calculated total energy distribution for four different p-doped cathodes. In order to see the doping effect more clearly, we assumed a VL position of

-0.5 eV and a potential barrier of 4 eV height and 1.5 Å width [6]. The effect of the different p-doping on the total energy distribution is remarkable. All the energies are referred to the baseline established by the bulk Conduction Band Minimum energy, with the result that the lower the p-doping level, the wider the total energy distribution becomes. This is mainly due to the change in the band bending width with the p-doping level. During all calculations, we assummed a constant electron mean free path of ~40 Å. The lower the doping level, the wider the band bending region, and thus the larger the number of scattering events undergone by the electrons.

On the other hand, Figure 4 shows the influence of the p-doping on the electron transverse energy distribution is almost negligible. The energy shown here is kinetic energy, and it is referred to the VL energy. The Average Transverse Energy (ATE) calculated is very small (~10 meV), and is independent of the amount of scattering suffered by the electrons. The mass effect is mainly responsible for this behavior. The energies involved in our problem are so small that the mass effect is dominant, so that the influence of the electron-phonon scattering on the final transverse velocity of the electrons is almost negligible.

The distributions plotted in Figure 4 show that, under the perspective of an ideal model, the GaAs NEA cathode would be an extremely high brightness electron source, where practically all the electron kinetic energy is directed normal to the surface.

In the experiment, when the electrons leave the cathode, they are accelerated toward a GaAs CCD. The spot size on the CCD surface is a function of the initial transverse velocity of the electrons when they leave the cathode and of the bias applied between cathode and CCD. For the case of a bias voltage, V >> ATE, the landing distance of the electrons to the central point (radius r) is given by

$$r = 2L(ATE\ /V)^{1/2} \tag{4}$$

where L = 1 mm is the distance between the cathode and the CCD array. Figure 5 shows the calculated spot size plotted against the experimental spot size obtained with the experimental set up described in Figure 1, using a bias voltage of 1000 V. With an experimental average transverse energy of ~100 meV and a calculated average transverse energy of ~10 meV, the big difference between the spot sizes is not surprising.

2. DISCUSSION

The mismatch between experiment and a simplified theory of electron emission from NEAs is an old problem [8,9,10]. As indicated in the previous section, the assumption of an ideal semiconductor-vacuum interface is at the root of this problem. Several authors have looked for a solution by modeling the emission from *rough* interfaces [3,11]. Other authors have assummed some type of periodical spatial structure at the interface [12], so that the conservation laws were effective locally, and Eq. (2) was transformed into a more complex expression.

Our guess is that this type of description is still too simple, so we approach the problem from other directions. We first consider the possibility that there is some scattering in the Cs,O layer. The electron angular distribution will be perturbed if some photoelectrons are scattered while they are crossing the Cs,O layer.

In Section 2.1, we present the calculated results for isotropic or cosine distributed scattering, and for Rutherford scattering, and then compare the results with the experimental data.

In Section 2.2, we make our model conform more closely to the experimental data by changing the electron effective mass inside the semiconductor, while maintaining the ideality in the interface by imposing the conservation laws during the emission. The physical meaning of this is not clear, but does give us important insights into the emission process.

2.1 SCATTERING IN THE CS,O LAYER

Little is known about the Cs,O layer. However, it has been reported [12] to be an amorphous layer and a strong electron scatterer .We modeled the scattering in the activation layer using the number of electrons which undergo scattering as our fit parameter. We compare our calculations with data from the experimental setup described in Figure 1. The GaAs cathode used was a typical transmission mode, high-yield cathode similar to that used in a standard night vision system. Bias voltages of 1000 V, 2000 V, and 3000 V were used during this experiment. We fitted the experimental spot for one of these bias voltages, typically 1000 V. Using the distribution obtained and Eq. 4, we calculated the spot size for the rest of the bias.

Figure 6(A1) shows the experimentally obtained spot size compared with the calculated spot size for isotropically distributed scattering in the Cs,O layer. The best fit corresponds to the case in which ~68% of the electrons are scattered. Scattering coefficient is indicated in the plots by SC. Figure 6(B1) shows the electron transverse energy distribution obtained for this case. Because of the long tail in the energy distribution, the spot shape is a brilliant central point with side wings. Figure 7, curves b, shows the evolution of number of electrons inside the central, side, and corner CCD pixels as a function of bias voltage. The differences obtained at high voltages is a direct consequence of the energy distribution shown in Figure 6(B1). This type of distribution concentrates a smaller amount of electrons in the CCD central pixel than the experiment showed overall for high voltages, while the electron concentration at the corner and side pixels is overestimated (see Figure 7, curves a).

Figure 6(A2) shows the spot size calculated for a cosine-distributed electron scattering in the Cs,O layer, compared with experiment, for a bias of 1000 V. The spot shape is similar to that for isotropic scattering, but the wings are shorter. The best fit corresponds to a scattering coefficient of ~80%. Figure 6(B2) plots the corresponding electron transverse energy distribution. Again the tail in the distribution is the cause of the small side wings. (Figure 7, curves c, shows that, even though there is not a bad fit to the experimental data, there are still too many electrons in the side and corner pixels when the bias voltage is high.)

Figure 6(A3) shows the calculated spot for a Rutherford-type scattering in the Cs,O layer compared with the experimental spot size. The best fit corresponds to a impact parameter of 3.5 Å and an ion charge of 1 e for an applied bias voltage of 1000 V. Figure 6(B3) plots the electron transverse energy distribution corresponding to this fit. Even though there is a good fit for a bias of 1000 V, we can see in Figure 7, curves d, that this type of distribution concentrates too many electrons in the central pixel. When the applied bias increases, the number of electrons in the central pixel also increases (although not as much as predicted by the calculation, which is overestimated) while the resulting number of electrons in side and corner pixels is smaller than shown by the experiment (curves a).

2.2 THE MASS EFFECT

As explained in Section 1, assumming an ideal semiconductor-vacuum interface has huge consequences on the calculated electron transverse energy distribution for GaAs. As Eq. (2) suggests, we can weaken this effect in our computer simulation by changing the effective electron mass inside the emitter. Figure 8 shows the magnitude of this effect. The parameters used for these calculations were: p-doping level 2×10^{19} cm^{-3}, temperature

300°K, VL –0.5 eV, and a TC corresponding to a triangular barrier with 4 eV height and 1.5 Å width. The electron total energy distribution does not depend on the electron effective-mass. However, the ratio between the number of electrons which reach the band-bending region and the number of electrons which finally get out (Escape Probability, EP) does. This dependence results from Eqs. (1) and (3). The smaller the effective mass, the larger the energy transferred from the transverse direction to the longitudinal direction [Eq. (3)], and the larger the number of electrons that satisfy Eq. 1. On the other hand, the mass effect on the electron transverse energy is remarkable. The ATE increases an order of magnitude when the internal electron effective-mass is increased from its value in the GaAs Γ valley to its value in vacuum.

Figure 9 shows the calculated spot size for the electron transverse energy distribution corresponding to m* = mo [Figure 7(d)] compared to the experimental spot size for a bias of 1000 V. This is our best fit to the experimental spot size—better than those obtained in the previous section, which assumed electron scattering in the Cs,O layer. As shown in Figure 7, curves e, correspond to this case, which is the best fit to experimental curves,.We can conclude that the calculated transverse energy distribution shown in Figure 8(D) must be very close to the real distribution.

We have compared our calculations with other experiments. Baum et al. [14], used a plate parallel dinode configuration with a spatial resolution ~10 μm, superior to the CCD experiment. The cathode was a semitransparent, high-yield GaAs cathode setting in a vacuum tube. Figure 10 compares our calculated with Baum’s experimental transverse energy distributions. Using the same electron effective-mass inside the semiconductor and inside the vacuum again results in good agreement between experiment and calculation.

Figure 11 shows the calculated angular distribution for two different effective masses inside the semiconductor. Theta is the angle between the electron direction when it leaves the semiconductor and the normal direction. As explained above, the distribution corresponding to $m^* = m_0$ must be close to the real distribution. Even when the mass effect is not considered in the calculation, and the *refraction effect* is smaller than theoretically expected, most of the electrons escape in the forward direction. Almost 75% are emitted in a cone of 40°; thus, the brightness of GaAs cathodes is high. This is because the kinetic energy gained by the electrons in the normal direction inside the band-bending region, ~0.5 eV, is much higher than the typical energies involved in our problem. However, the brightness could be orders of magnitude higher using $m^*=0.067\times m_0$, rather than $m^*=m_0$, maintaining ideality in the interface, as shown in Figure 11b where more than 80% of the electrons are in a cone of 15°.

Figure 12 plots the calculated ATE versus electron effective-mass curves for several VL positions. The smaller the electron effective -mass used in the calculation, the smaller the dependence of ATE on the VL. For electron effective-masses smaller than $0.1\times m_0$ we can consider ATE VL independent. Experimental evidence indicates that ATE depends directly on the Quantum Efficiency of the cathode [5,13]—the higher the Quantum Efficiency, the higher ATE. Quantum Efficiency is directly related to the VL position; we can assume that, under the same experimental conditions, a change in QE is due to a change in the VL position. If the mass effect were present, we would not expect to see any important change in the ATE, but this is not the case—the experimental variation of ATE with QE is remarkable. This is further evidence that the real case differs from the ideal case. Unfortunately, we do not have quantitative experimental data to fit this variation. However, some previous results [14] do seem to indicate that, again, the curve corresponding to $m^* = m_0$ must be very close to the experimental data.

Conclusions

We have shown that a simplified theory that assumes emission from an ideal semiconductor-vacuum interface cannot explain the large average measured electron transverse energy of electrons emitted from NEA GaAs cathodes. The three electron scattering mechanisms in theCs,O layer (isotropic, cosine, and Rutherford scattering), do not fit the experimental data very well. We find that, in general, a model in which some electrons undergo isotropically or cosine distributed scattering at the activation layer ,while others escape without any interaction, is not an adequate description of the mechanism for the electron transverse energy spread. In fact, if that were the case, we would expect to get spots with a brilliant central point and long side wings, in disagreement with experimental evidence. On the other hand, Rutherford scattering does not fit the experimental data, either— it concentrates too many electrons in a small zone, with a calculated emission cone that is smaller than the experimental one .

The best fit to the experimental data corresponds to the case that assumes the electron effective-mass inside the semiconductor is equal to the electron effective-mass in the vacuum. The electrons behave as if they have lost their *memory* and forget where they are from when they are released at the Cs,O layer. What this really means is difficult to understand. The Cs,O layer is an amorphous layer, which plays a key role during the emission process. The conservation of the transverse crystal momentum during the emission from a crystal to an amorphous material is probably too strong an assumption. This is the root of the experiment-calculation mismatch. The interesting point here is the evidence that the experimental data are best-fitted, equaling the electron effective -mass inside and outside the semiconductor. It will be necessary to do a deeper theoretical study of the electron emission in a crystal-amorphous interface. A best knowledge of the rules in this type of system will give us important information for improving Negative Electron Affinity devices.

Results of this study indicate some directions for improving the actual performance of NEA cathodes: the study of new activation methods in order to get less amorphous layer and the study of new materials with smaller effective electron masses.

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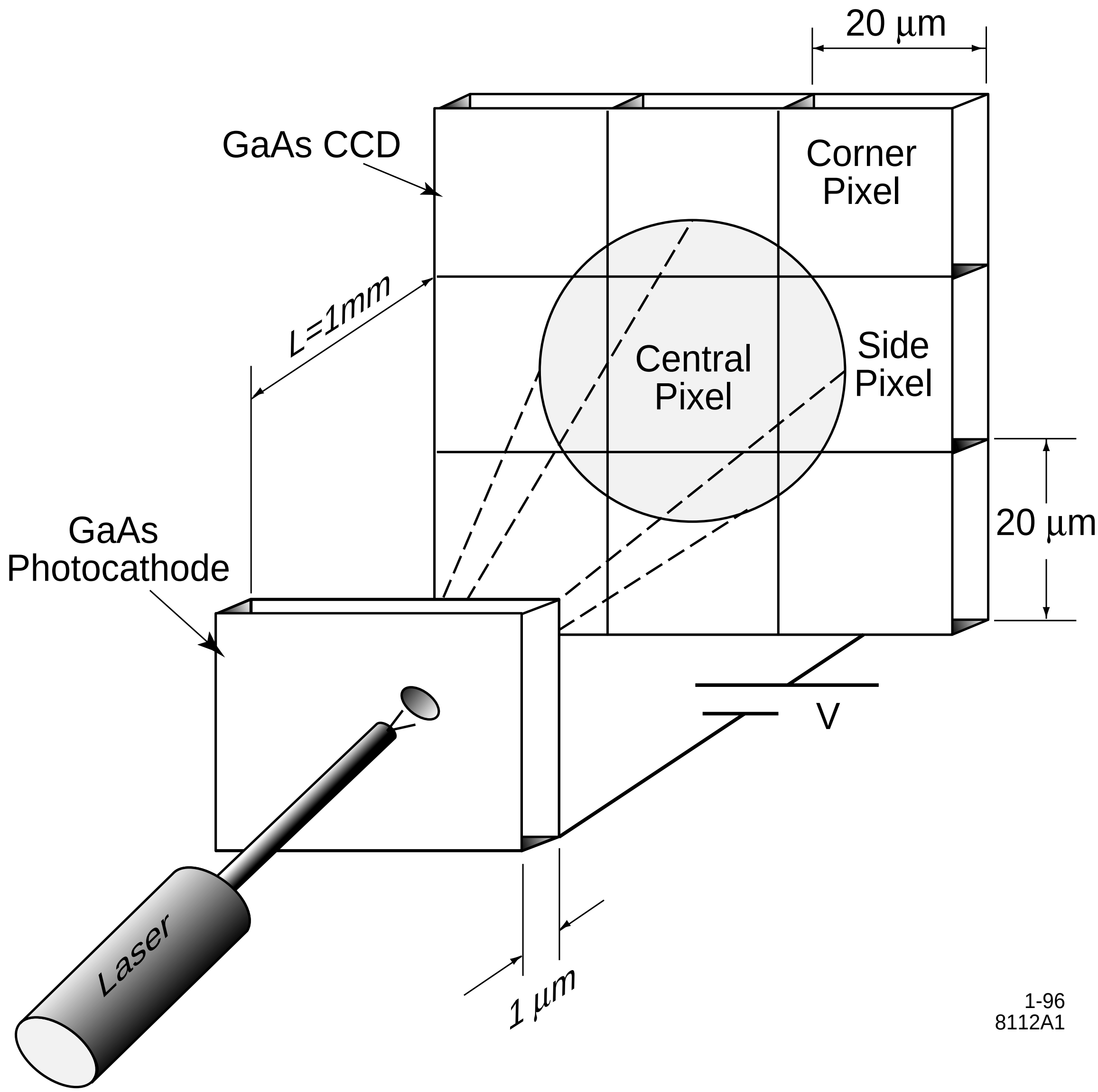

Figure 1. Experimental set up used for measuring the electron transverse energy distribution for a transmission mode cathode. The light source was a He-Ne laser. The initial spot size was ~4 μm on the cathode's back side. The cathode was a AlGaAs/GaAs:Cs,O high yield cathode typically used in night vision devices. The spatial resolution was mainly limited by the CCD pixel's size (~20 μm).

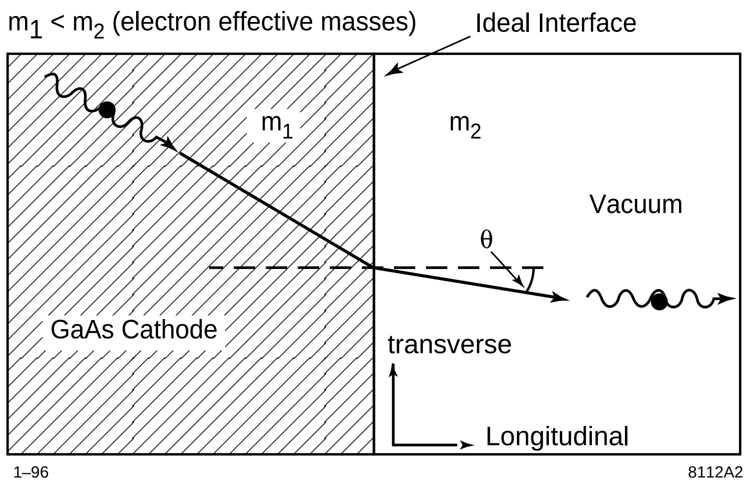

Figure 2. The mass effect picture. Because of the different electron effective mass inside (m_1) and outside (m_2) the semiconductor, during the electron emission and assuming ideal interface, the electrons suffer a *refraction* or change in their direction. If $m_1 > m_2$, then $\theta_1 > \theta_2$. The deviation is proportional to the difference in the effective electron masses.

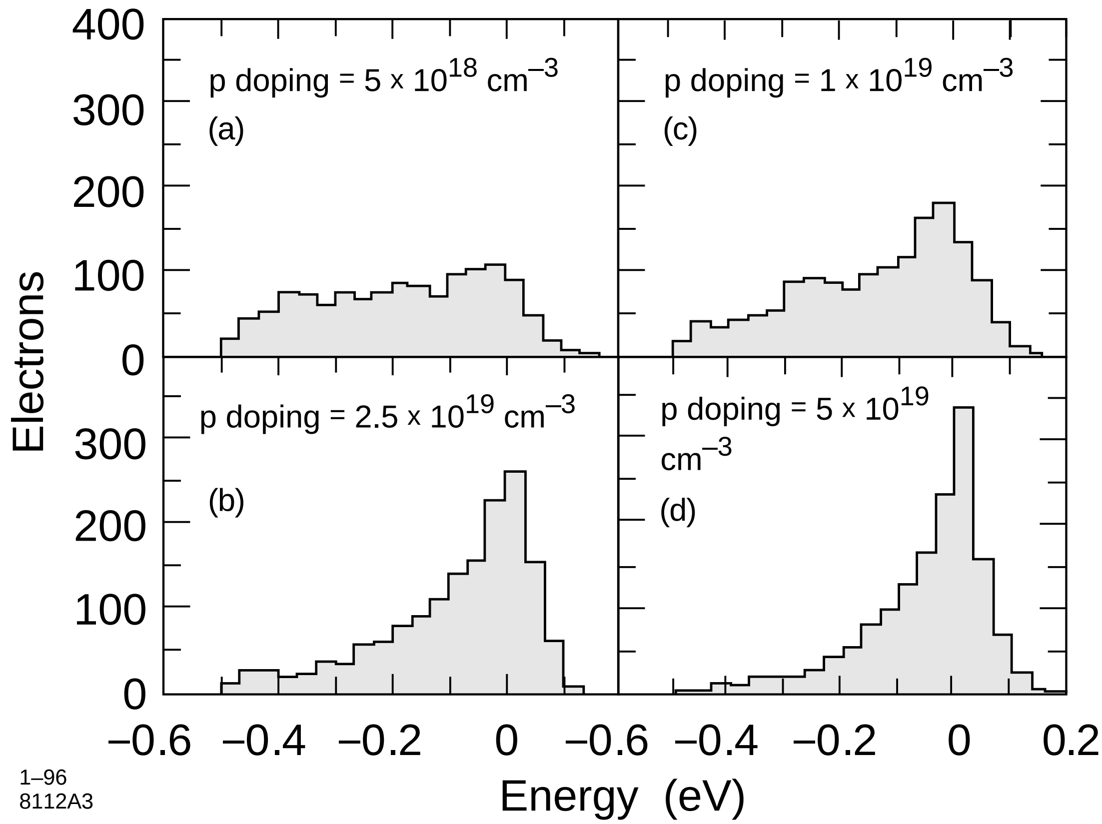

Figure 3. Calculated Electron Total Energy Distributions for four different p-doping levels of a transmission mode GaAs photocathode. The parameters used in the calculations were: temperature, 300 K; VL position, -0.5 eV; effective electron mass $m^* = 0.067 \times m_o$; and a Transmission Coefficient corresponding to a triangular barrier of 4 eV height and 1.5 Å width. The energies are referred to the bulk's CBM. The Escape Probability (EP) is the ratio between the number of electrons which reach the band bending region and the number of electrons which get out to the vacuum.

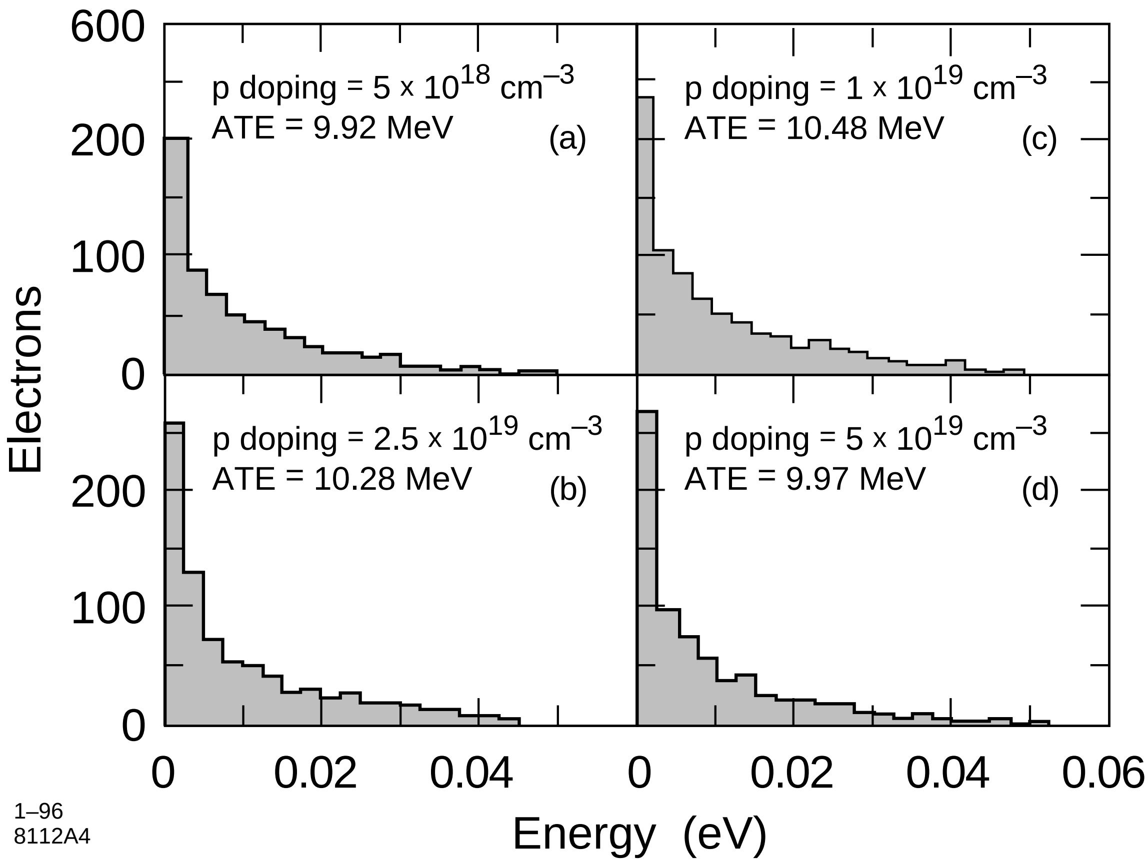

Figure 4. Calculated Electron Transverse Energy Distributions corresponding to the same conditions described in Figure 3. The energy is referred to the VL. The Average Transverse Energy (ATE) is independent of the p-doping level is a direct consequence of the mass effect, which screen the effects of having more scattering as the p-doping concentration is lower.

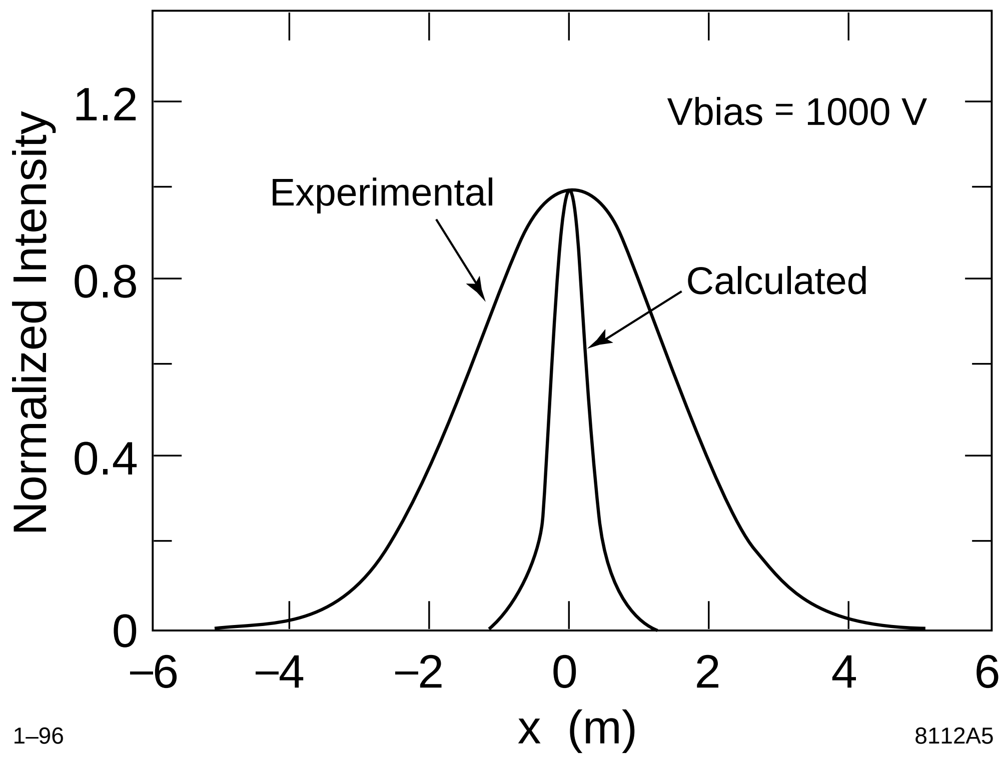

Figure 5. Experimental and calculated spot on the GaAs CCD described in the experimental setup in Figure 1. The bias was 1000 V and the cathode doping level was 2×10^{19} cm^{-3}. The experiment-calculations mismatch is mainly due to the assumption of ideal semiconductor-vacuum interface.

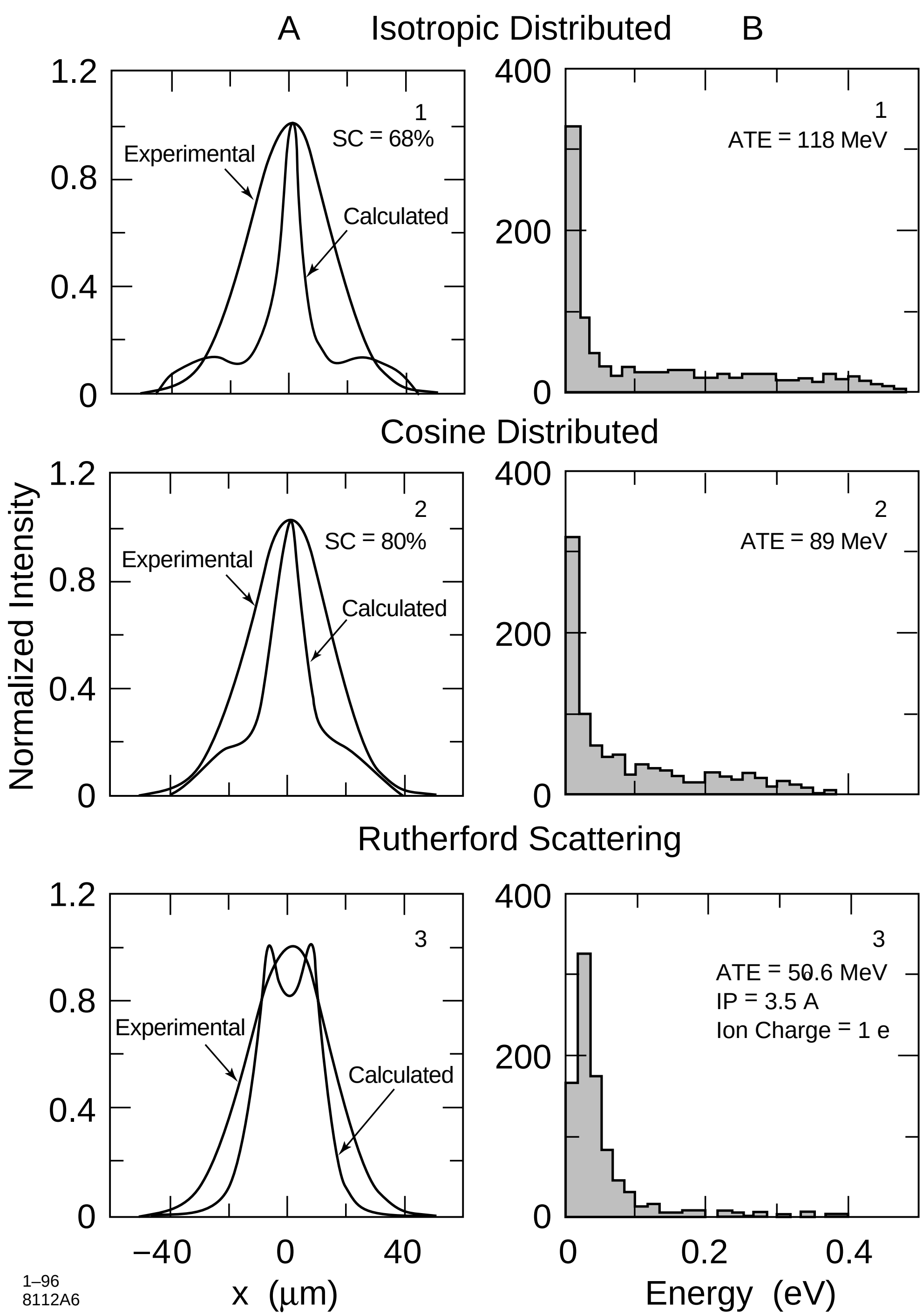

Figure 6. (A) Experimental compared to calculated spot on the GaAs CCD in the case where it is assumed that some electrons are (1) isotropically, (2) cosine, or (3) Rutherford scattered in the Cs,O layer. The scattering coefficient SC is the percentage of electrons that have been scattered while they cross the Cs,O layer; it is used as a fitting parameter. The spots correspond to a bias of 1000 V. (B) Electron Transverse Energy Distributions corresponding to the cases described in (A). The Average Transverse Energy (ATE) for each distribution is also shown. The long tails in Cases 1 and 2 are responsible for the side wings in the spots plotted in (A1) and (A2).

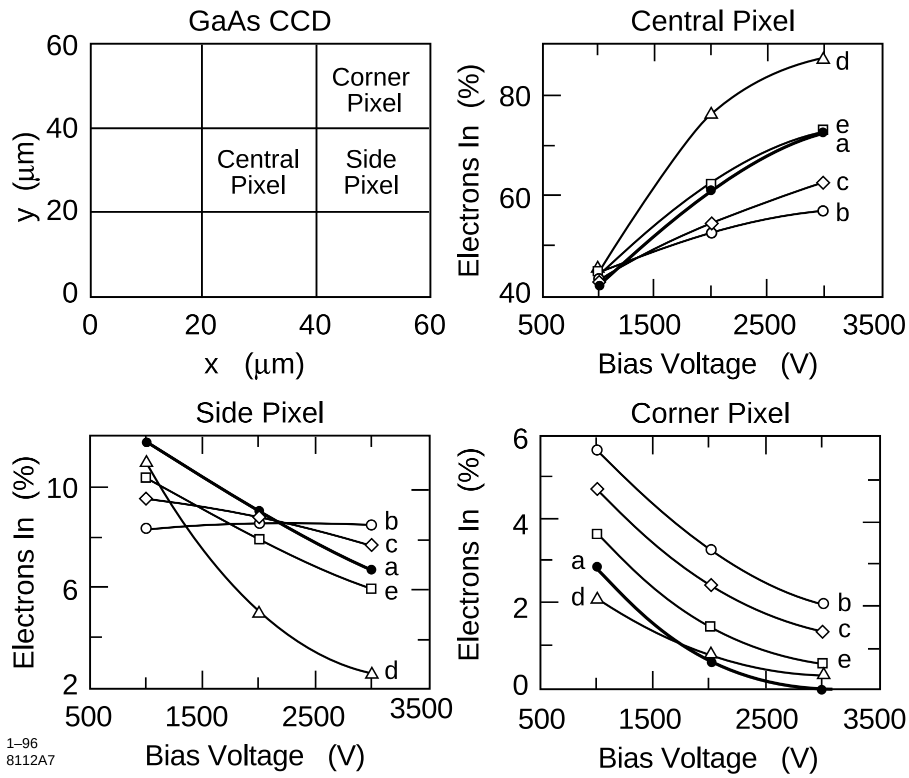

Figure 7. Evolution of the percentage of electrons inside the central, side, and corner pixels with the bias voltage for: (a) experimental; (b) isotropic scattering; (c) cosine scattering; (d) Rutherford scattering and (e) effective electron mass approximation ($m^* = m_o$). The best fit corresponds to curves (e) where it has been assumed that the electrons inside the semiconductor have the same effective mass as those in the vacuum.

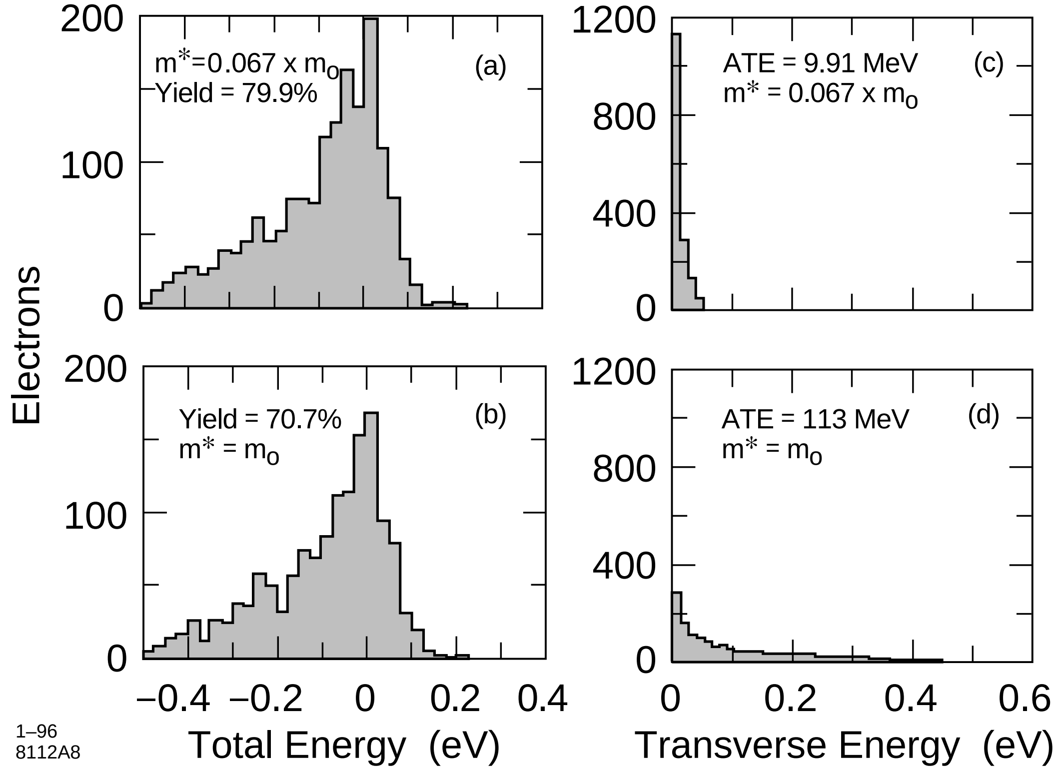

Figure 8. The mass effect on the total energy distribution and on the transverse energy distribution. The calculated distributions shown here correspond to a p-doping level of 2×10^{19} cm^{-3}, temperature 300 K, VL = -0.5 eV, TC associated with a triangular barrier of 4 eV height and 1.5 Å width with (1) $m^* = 0.067\times m_o$ and (2) $m^* = m_o$. The total energy is referred to the bulk's CBM, and the transverse energy is referred to the VL. The escape probability EP is the ratio between the electrons which reach the band bending region and the electrons which, finally, can get out.

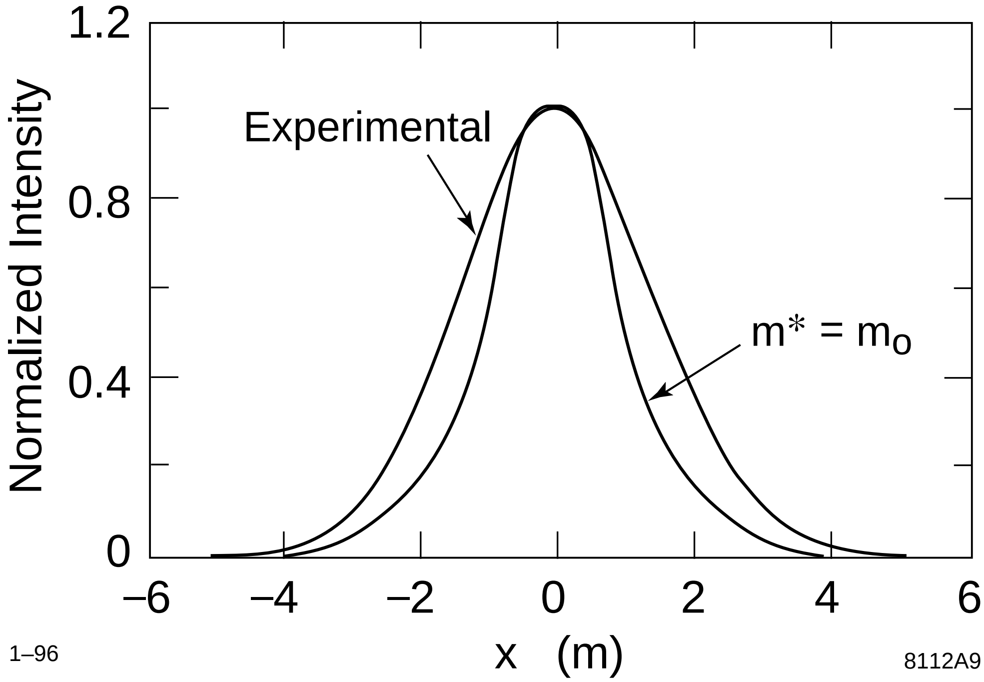

Figure 9. Experimental spot size compared with calculated spot size in Case 2 in Figure 8. This is the best fit that we obtained. It corresponds to 1000 V bias between the CCD and the cathode.

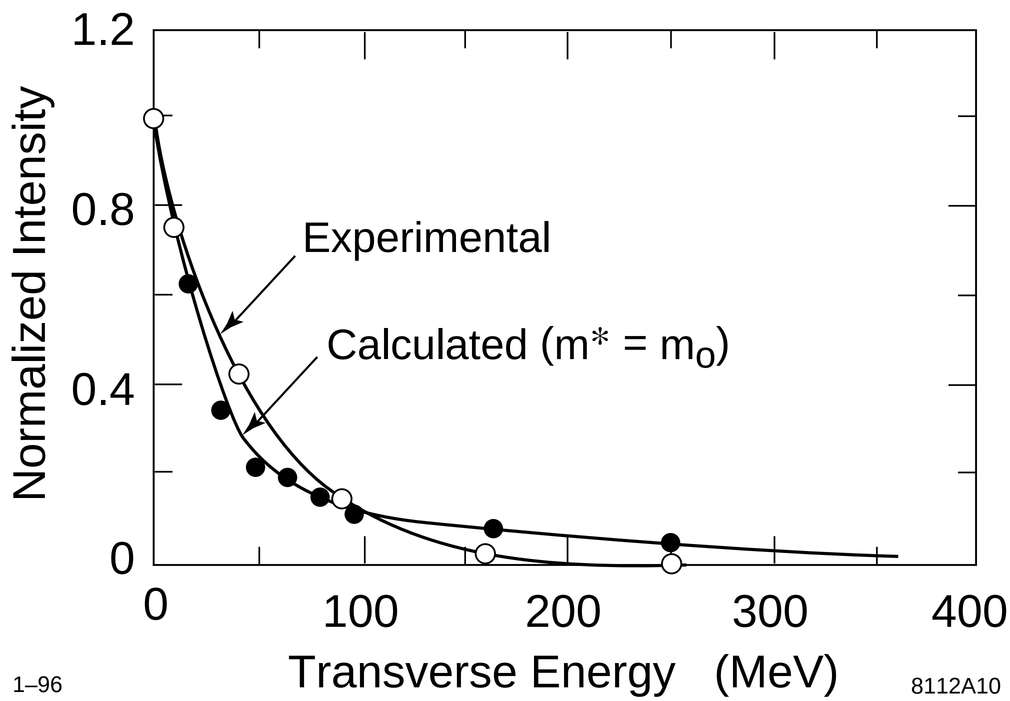

Figure 10. Comparison between the calculated and experimental transverse energy distribution. The experimental data correspond to a dinode configuration experiment described in Ref. [12]. The calculated data are the same as shown in Figure 8 (2). Again, this corresponds to the case where $m^* = m_o$.

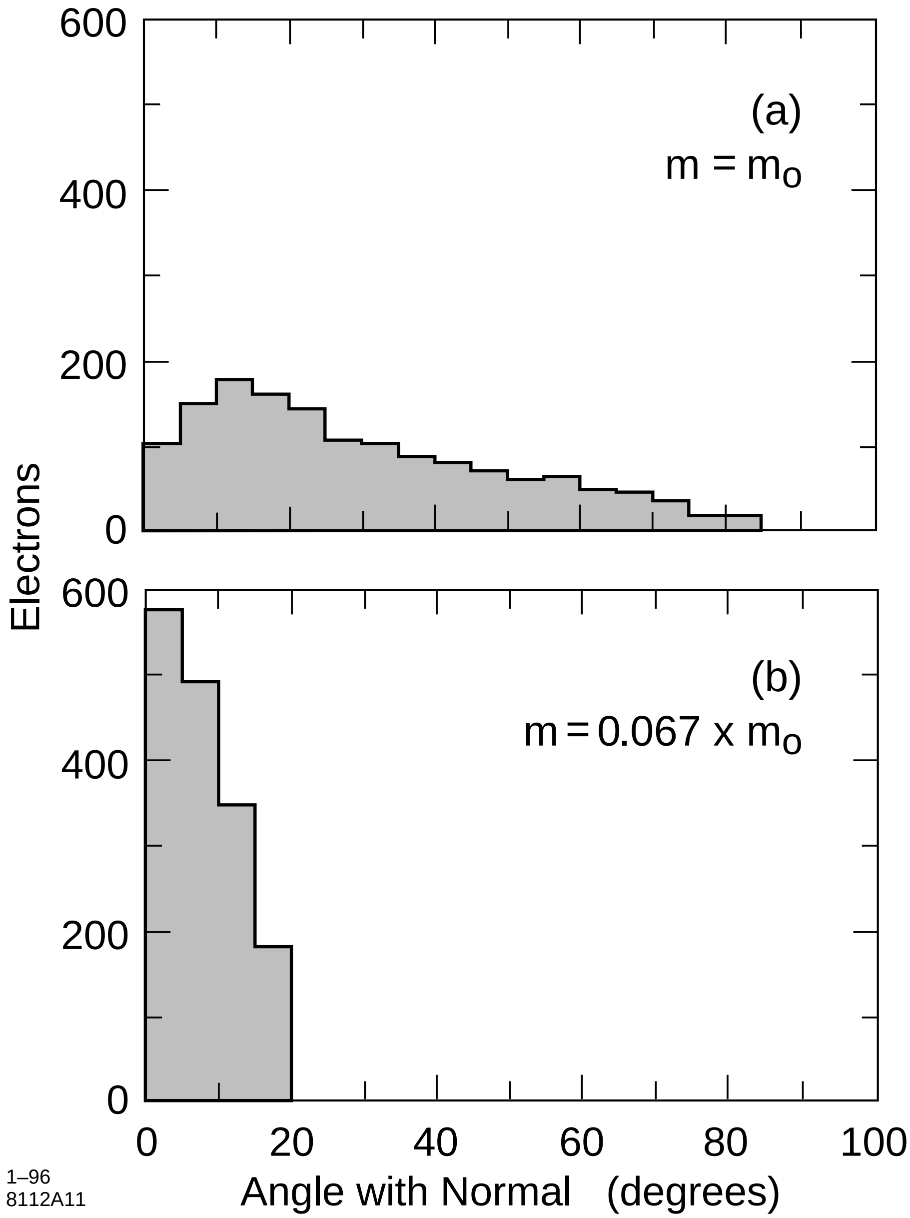

Figure 11. Calculated Normal Angle Distribution for two different effective electron masses. Assuming m* = m_0, close to the experimental evidences, that ~75% of the electrons are getting out in a cone of 40°, giving a very high brightness. In the case of an ideal interface, the brightness is several orders of magnitude higher. We can see that having a good interface is essential in order to improve the characteristics of the electron beam.

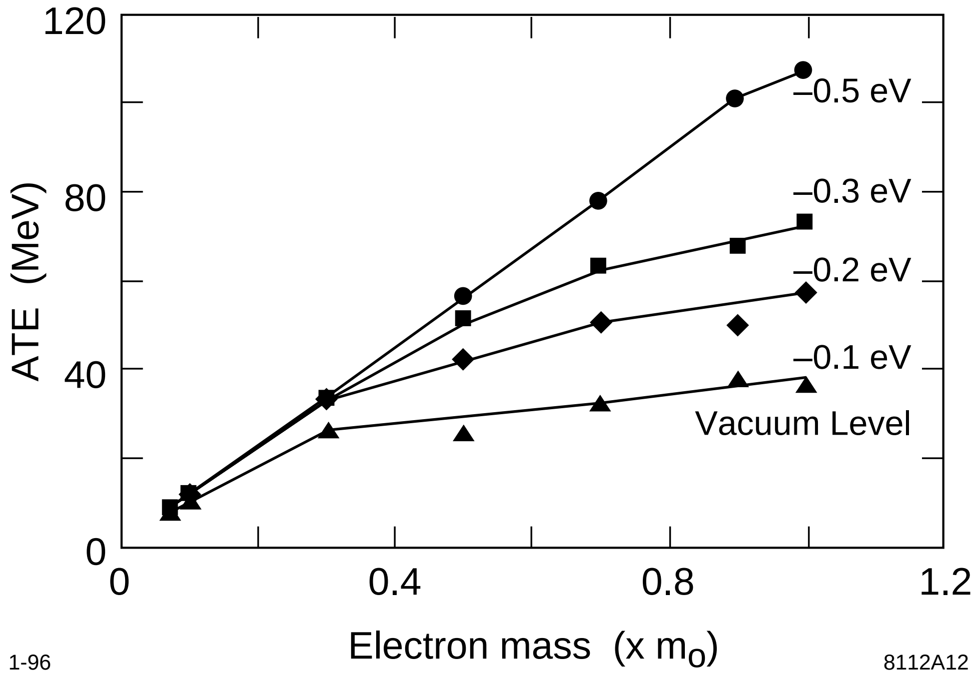

Figure 12. Calculated Average Transverse Energy (ATE) evolution with the effective electron mass for several VL positions. The calculations were done assuming a p-doping level of 5×10^{19} cm^{-3}, a 300°K temperature, and a TC with a triangular barrier of 4 eV height and 1.5 Å width. The lower the effective electron mass, the smaller the variation of the ATE with the VL position—for an effective electron mass smaller than $0.1\times$m