Spectral Response of GaAs(Cs, NF_3) Photocathodes

Teresa Esposito
tesposito2009@my.fit.edu
Florida Institute of Technology

August 10, 2012

ABSTRACT

In order to study the spectral response of GaAs(Cs, NF_3) photocathodes, Quantum Efficiency was measured as a function of incident photon energy and compared with Monte Carlo simulations. Experimental data has been taken on two different photocathodes after they have been activated and as they are "dying". Monte Carlo simulations of activated GaAs have been done with different electron affinity while the photon energy is being varied. A comparison of experiment and simulation is promising, although more work on the simulation is being done.

1. Introduction

Photocathodes are a subject of great interest as a source of electrons of a high brightness beam. Cornell's Energy Recovery Linear Accelerator Injector (ERL) is using such cathodes for its prototype, however, the detailed physics that explain many of the fundamental properties of photocathodes such as Quantum Efficiency (QE)-the number of electrons emitted per incident photon- , energy distributions, and response time are still not well understood. GaAs cathodes activated to negative affinity with Cs and NF_3 are an important class of photoemitters due to their intrinsic high brightness and high QE. [1]. GaAs cathodes are being used because of their low Mean Transverse Energy (MTE)- average energy perpendicular to the surface normal. One important requirement for making a photocathode is the vacuum in which it is made and stored in. Without vacuum (mainly of water vapor and Oxygen which are responsible for "poisoning" of the Cesium layer) in the 10^{-12} Torr range, the cathode's QE will decrease rapidly, rendering it useless. In order to keep the cathode in the best vacuum possible, all of the different chambers where tests, growth, and activation occur are connected together. This way, the cathode can be moved from chamber to chamber via magnetic translator arms. A model of the vacuum chamber can be seen in Figure 1.

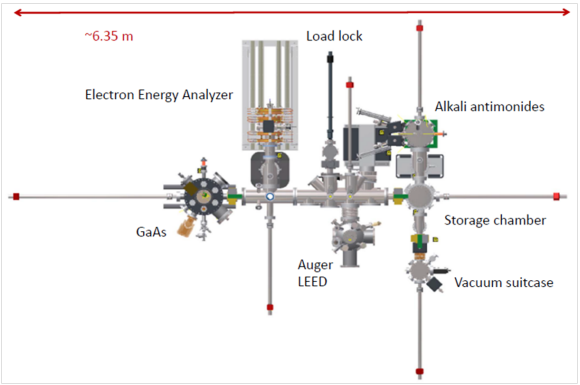

Fig. 1.— Illustration of the vacuum chamber used for both making and studying photocathodes.

Electrons are released from the cathode via photoemission. The photoemssion process can be described as a three step process, illustrated in Figure 2. First, the electrons are exited from the valence band into the conduction band. Then, the electrons will diffuse to the surface. Finally, they can be emitted into the vacuum [2]. In order to understand this process, a Monte Carlo simulation is being developed in order to track the position and momentum of each electron from within the bulk until they are released from the surface[4]. This simulation also must incorporate information about the surface of GaAs once it is activated. This includes band bending at the surface and a barrier at the surface-vacuum interface, among other things. One interesting feature that can be studied using this code is the dependence of QE on the incident photon energy. In order to do this, the simulation can be run multiple times with different incident photon energies and corresponding absorption lengths. This relationship can also be measured experimentally using a monochromator to directly scan through different wavelengths of incident light on the cathode while continuously measuring photocurrent.

This paper will first describe the basic theory behind spectral response of GaAs. Then, the activation process of two different cathodes and RHEED measurements before and after activation will be described. Next, the experimental spectral response results will be presented. Finally, the Monte Carlo simulations that were performed using different incident photon energies and surface barrier will be given, followed by the conclusion.

2. Spectral Response Theory

A theoretical idealized relationship between incident photon energy, hf, and QE can be described by

$$QE(hf) = \frac{B[1 - R(hf)]}{1 + [\alpha(hf)L]^{-1}}, \qquad (1)$$

which is obtained using a diffusion model of electrons in GaAs[3] . This equation assumes that the incident photons create a thermalized distribution of electrons and does not take into account the surface barrier, band bending region, or scattering that electrons undergo. In this formula, R is optical reflectivity, α is the optical absorption

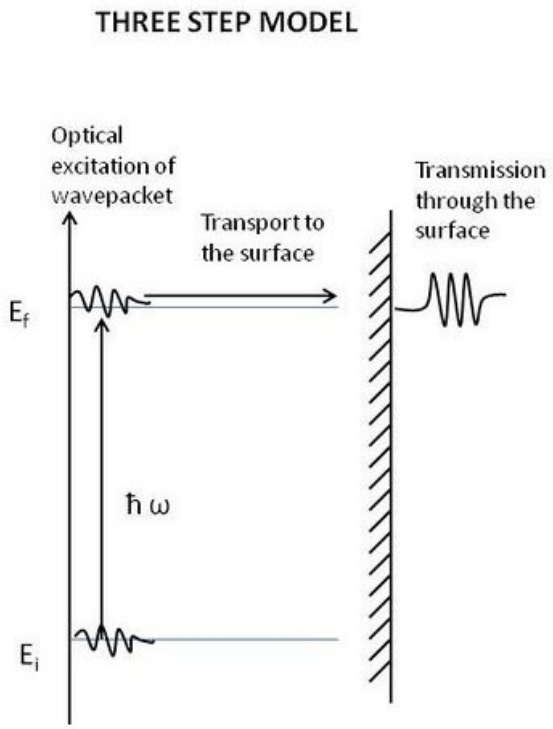

Fig. 2.— The three step model of photoemission [1].

coefficient, L is the electron diffusion length, and B is the surface escape probability. L and α are properties of bulk GaAs while R is a property of a GaAs surface. B, however, is a property of the particular cathode's surface, and hence will be dependent on cleaning and activation of the cathode.

3. GaAs Experimental Samples

Two different GaAs samples have been used in order to study Spectral Response. Sample 1 is p-doped using Zinc, with a doping level between $6.3x10^{18}$ and $1.9x10^{19}$ holes/cm^3. The wafer was cut from a 4 inch diameter commercial GaAs crystal using a laser. It was then cleaned in acetone and trichloroethylene to remove any contaminants from the surface. Then, the wafer was anodized in dilute phosphoric acid, creating an anodized layer 50 nm thick. Just before the wafer is indium soldered to the puck, the anodized layer is removed using ammonium hydroxide. Once under vacuum, the cathode was heated to about 600°C in order to clean off any residual Carbon contaminants and surface oxides.

Sample 2 (G20219), was made with epitaxially grown GaAs under UHV. Only the top 1000 nm of the sample was p-doped with Carbon at a doping level of $2.0x10^{18}$ holes/cm^3. After it was grown, an Arsenic cap was deposited onto the surface, allowing the GaAs surface to be sealed off from air and transported from the molecular beam epitaxy growth lab to the cathode system. The initial heating of this cathode was to 300°C which is when the As will evaporate off of the surface, leaving it atomically flat and clean. Activation, Reflective High Energy Electron Diffraction, and Spectral Response measurements have been taken for both of these cathodes. We also have the capabilities to perform Auger Spectroscopy and Low Energy Electron Diffraction, but have not yet done so at this time.

4. GaAs Activation

On its own, GaAs does not emit electrons in the visible light range. Plain GaAs is a positive electron affinity material, meaning that the vacuum level is higher than the conduction band minimum. In order to make use of GaAs, it must first be activated with Cesium and either Oxygen or Nitrogen Trifluoride gas. This will bring the vacuum level below the conduction band minimum by creating a strong field due to a dipole layer formed by a rough monolayer of Cs donating its electrons to the p-doped bulk. This means that an electron only needs to have enough energy to reach the valence band, and then can be released from the cathode without any extra energy. Activation of GaAs still has several aspects which remain poorly understood.

The technique we used to activate GaAs is Yo-yo activation. A clean cathode is first sprayed with Cs until the QE passes a maximum and goes down to about half of the maximum reached. Then, either O_2 or NF_3 is sprayed until the QE reaches another maximum. Cs is sprayed again, and the process repeats until each consecutive maximum does not have a significant increase in QE. Figure 3 shows an activation of Sample 1 with Cs and NF_3 gas. The maximum QE reached in this activation was 11%, and the 1/e lifetime was about 80 hours. Figure 4 shows a similar activation of Sample 2. The maximum QE reached was 4.2%, and the 1/e lifetime was about 25 hours.

5. Reflective High Energy Electron Diffraction

RHEED is used to study the surface crystal structure. It consists of shooting an electron gun at the cathode and observing the diffraction pattern that is created. This was done with electrons of energy 5.7 keV, and with the gun at a very shallow angle with the surface. For an atomically flat surface, the RHEED pattern is expected to be long vertical lines. When the surface is rough or oxidized, the pattern will change from lines to dots.

Figure 5 shows the RHEED patterns that have been taken after cathode cleaning and after activation of Sample 1. Between these two measurements, the cathode was locked in the same position, so that the RHEED pattern would be of the exact same position on the surface. Both RHEED patterns show the exact same spots on the surface. Figure 6 is a similar picture for Sample 2. The cathode was not locked in the same position during the measurement, but the RHEED patterns show almost the same lines in roughly the same position. These results confirm that Sample 2 has a much flatter surface than Sample 1. These results also

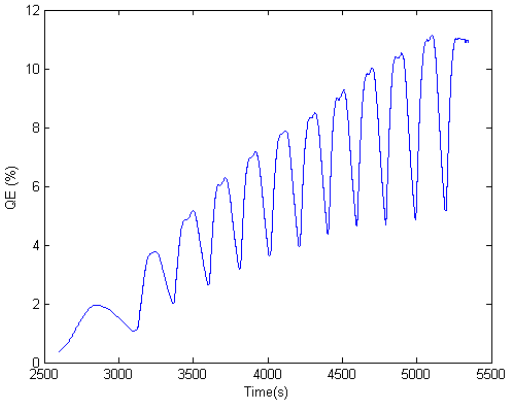

Fig. 3.— Sample 1 activation with Cs and NF_3 done on 8/1/2012.

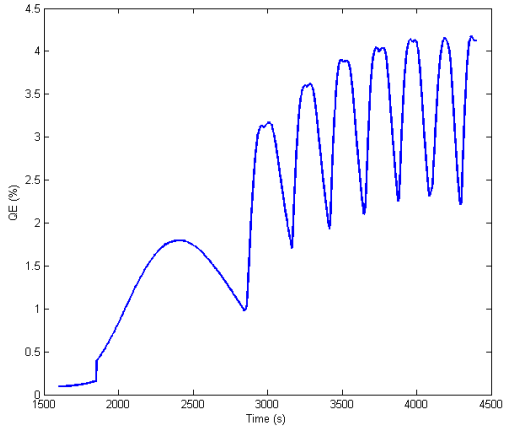

Fig. 4.— Sample 2 activation with Cs and NF_3 done on 8/5/2012.

show that before and after activation, the cathode surface remains relatively unchanged in terms of surface roughness. In both RHEED patterns after activation, the background light gets brighter while the dots and lines dim. This more diffuse pattern could be attributed to scattering off of the cesium layer.

6. Spectral Response

The experimental measurement of spectral response was done using a Newport monochromator (Model #70514) which screens out all but a small range of wavelengths from white light created by a mercury lamp. The QE is measured continuously while the monochromator outputs light from 350 to 1000 nm. The monochromator light beam passes through a Scitech optical chopper (Serial #5087) rotating at 1477 Hz and then a beam splitter, allowing measurement of light power throughout the QE scan. Photocurrent is measured by indirectly measuring the current created by photoemission. The signal is read by a SRS lock in amplifier (Model #530) which can lock into the chopper frequency, measure the current pulses and separate it from any background current. Both the raw photocurrent and light power is measured in LabView, and a Matlab code is used to process the results.

As the cathode dies, its spectral response will change. This is because as the cathode dies, its work function that was lowered during activation will change back to its original level. Conversely, the band gap energy of GaAs will remain the same even as the cathode dies. Once the affinity begins to become positive, even though electrons can reach the valence band, they are unable to escape because of the surface barrier and the QE drops off at a lower wavelength.

Selected spectral response curves are plotted in Figure 7 for Sample 1. These curves are taken over time to show the spectral response as the cathode dies. Because the death of the cathode was fairly slow, NF_3 was released in the chamber to raise the vacuum to the order of 10^{-7} Torr for a few seconds, killing the cathode much more rapidly. Figure 8 is a similar set of curves for Sample 2. This cathode was not killed with NF_3 because, as seen in Figure 9, the curves from Sample 2 behave like Sample 1 after it was exposed to NF_3. QE

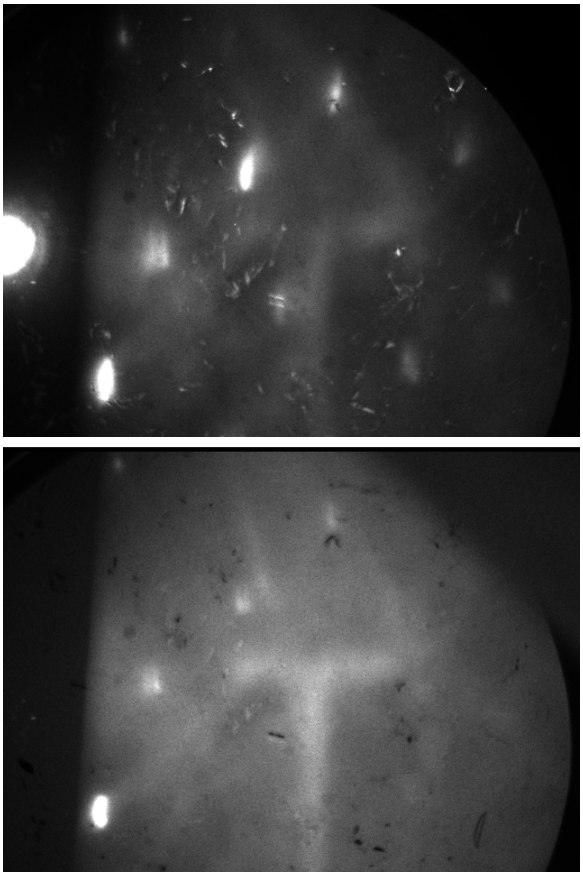

Fig. 5.— Top. RHEED done on Sample 1 before activation on 7/26/2012. Bottom. RHEED done on Sample 1 after activation on 7/30/2012. (The T shaped structure in the background of each picture is the reflection of the camera stand, and is not part of the RHEED pattern.)

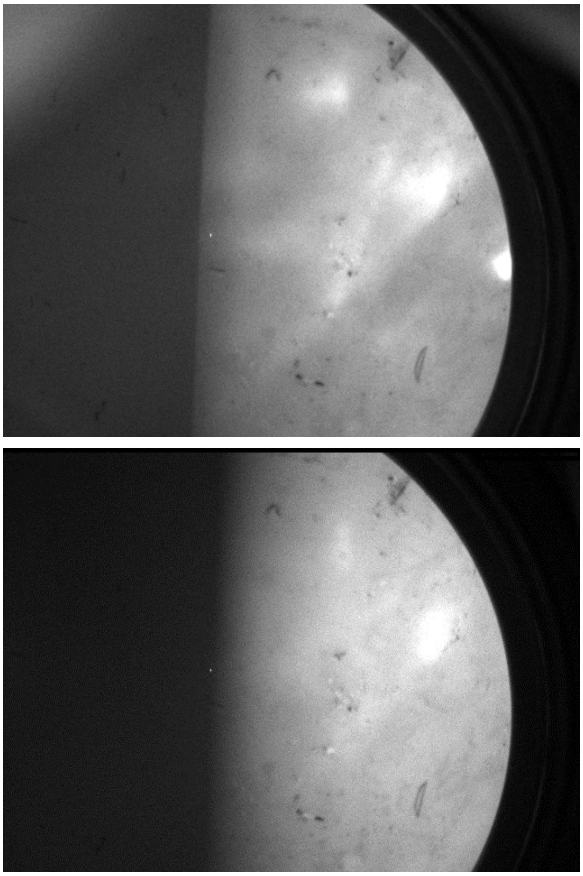

Fig. 6.— Top. RHEED done on Sample 2 before activation on 8/3/2012. Bottom. RHEED done on Sample 2 after activation on 8/6/2012.

in both of these cases drops off at a wavelength much lower than that corresponding to the band gap, meaning that the affinity is more positive.

These spectral response curves have also been compared to the theoretical model given in Equation 1. Because this model does not take into account things such as band bending, scattering, and a barrier, the curve given is oversimplified. Figure 10 shows that the theory only matches experimental data near the band gap, and only for cathodes that have reached negative affinity. If the cathode has a positive affinity, the theory does not explain the experimental data at all.

7. Monte Carlo Simulations

Since the exact mechanism of electron release in cathodes is still unknown, a Matlab code is being developed in order to simulate the flow of electrons during photoemission[4]. This code uses places electrons within the bulk as a exponential decay from the surface according to the laser penetration depth. Then, by using Monte Carlo simulations, these electrons undergo random scattering in the bulk due to impurities, phonons, and interactions with holes. This will cause the electrons to lose energy and eventually form a thermalized distribution, although they will not reach this distribution before reaching the surface. The electrons are tracked on their way through the bulk to the surface where a band bending region is simulated by an electric field. Both the conduction band minimum and the valance band maximum will bend downward, so that the Fermi Level of GaAs will be located at one third of the band gap. The surface barrier height is the difference between the conduction band minimum after bending and the vacuum level[4].

However, before the electrons can escape, there is also a higher triangular shaped barrier that they must tunnel through[3]. This barrier was added in the form of a set of finite rectangular barriers with heights that can adjust to form downward steps. The maximum barrier height and number of steps are defined by the user, and the steps will go from the maximum to the vacuum level. For these simulations the maximum barrier height is defined to be 0.28 eV above the surface barrier, and the number of steps was set to one, leaving just a rectangular barrier[3]. Different surface barrier heights

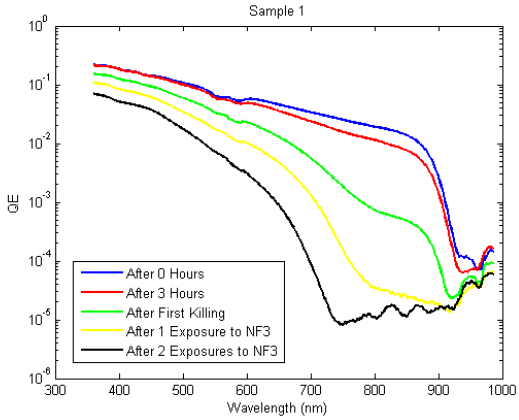

Fig. 7.— Experimental spectral response curves taken for Sample 1 on 8/1-2/2012. First killing refers to an unknown cause of bad vacuum inside the chamber which caused the cathode to die rapidly without the release of NF_3.

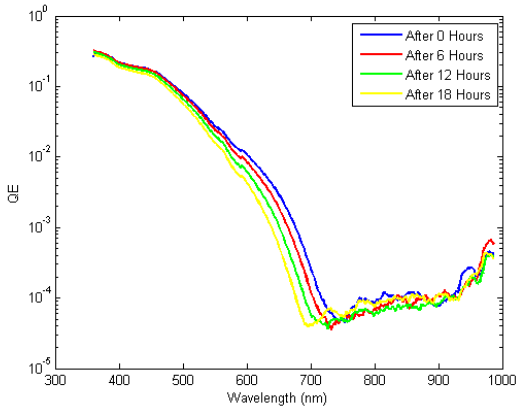

Fig. 8.— Experimental spectral response curves taken for Sample 2 on 8/5-6/2012.

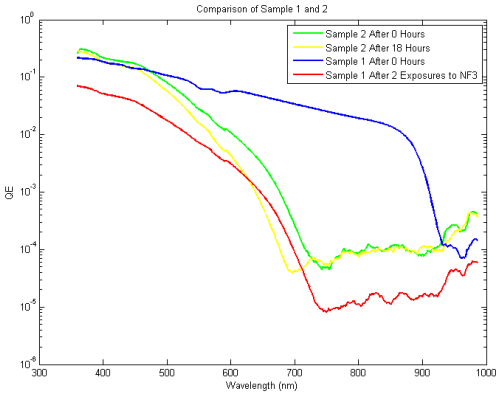

Fig. 9.— Comparison of the first and last spectral response curves for each cathode.

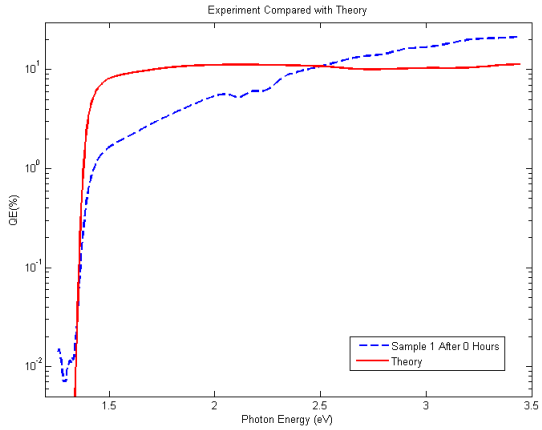

Fig. 10.— Comparison of the first spectral response curve taken of Sample 1 with the simple theoretical model given in Equation 1.

will translate to different electron affinities of the sample. Figure 11 shows a simulation plot of band bending and the surface barriers. Once the barrier is defined, the reflectivity of the barrier is calculated using a series of reflection matrices. This revised reflectivity is used to determine QE, MTE, time response, and other useful quantities.

Once these changes were made to the existing code, an more useful simulation can be done by running the code multiple times while changing one parameter. In this case, both the energy of incident electrons and the surface barrier was changed before each simulation. This way, the both the trend of the spectral response curve can be studied, and the surface barrier height can be identified.

Figure 12 plots the simulation curves that correspond best with the spectral response curves from Sample 1. The simulation describes the curves well until about 1.8 eV, which is when electrons are able to be exited into other valleys. The simulations are ongoing, and by changing the barrier and other values in the simulation, a better agreement can be reached. A second simulation has been done with all of the same parameters except using the doping level corresponding to Sample 2. These simulations did not follow any of the experimental spectral response curves obtained for Sample 2. The cause of this discrepancy is not presently understood.

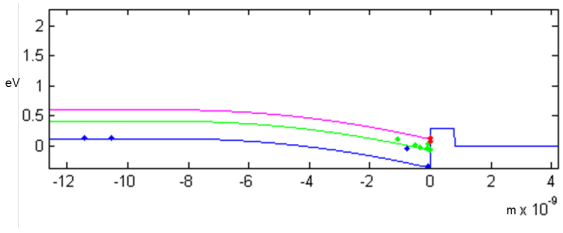

Fig. 11.— A figure created by the Monte Carlo simulations showing band bending and barriers. The blue curve corresponds to the Γ valley, pink is the X valley, and green is the L valley. Electrons are represented as dots, the color that they are corresponds to which valley they are in.

8. Conclusions

During this project, two p-doped GaAs(Cs, NF_3) photocathodes have been successfully activated using the Yo-yo activation procedure. RHEED has also been performed on both cathodes before and after activation. RHEED on Sample 1 indicated that the surface of the cathode was rough both before and after activation, although the background of the pattern taken after activation was brighter. This could mean that the Cs layer causes more scattering. The RHEED pattern for Sample 2 contained lines, meaning that it was flatter than Sample 1, and also showed a similar background brightness increase.

Through the spectral response investigation of these two photocathodes, a rough method for identifying the affinity of a cathode has been made. When a cathode has reached negative or near negative affinity, the band gap of the cathode can clearly be identified as a sharp drop in quantum efficiency on a log scale. Cathodes that are at positive affinity will have a slower drop at a much smaller incident photon wavelength. Using this approximation, the evolution of Sample 1's spectral response curves indicate that the cathode was at or near negative affinity soon after activation, and as time progressed (as the cathode died) reached positive affinity. However, these simulations do not fit the experimental data with incident photons above 1.8 eV. From the spectral response curves for Sample 2, it is clear that this activation did not bring the cathode to negative affinity. Using the Monte Carlo simulations, an affinity can be assigned to these spectral response curves.Investigations to find the cause for this discrepancy are still ongoing.

9. Acknowledgments

I would like to thank my advisors, Siddharth Karkare, Dr. Luca Cultrera, and Dr. Ivan Bazarov, for proposing and helping me complete my project. I would also like to thank everyone else in the ERL group including Eric, Tobey, Adam, Dr. Bill Schaff, and Dr. Xianghong Liu for their help. Finally, I would like to thank the Cornell Accelerator Physics Staff for running the REU program. This project was supported by the NSF REU grant.

10. References

[1] Photocathode Wiki, photocathodes.chess.cornell.edu/wiki/Cathode_theory

[2] W. E. Spicer, SLAC-PUB-6306 (1993)

[3] D. G. Fisher. J. Appl Phys., Vol. 43, No.9, September 1972

[4] S. Karkare, Photoemission Characteristics of GaAs(Cs,F) Photocathodes using Monte Carlo Simulations (Unpublished)

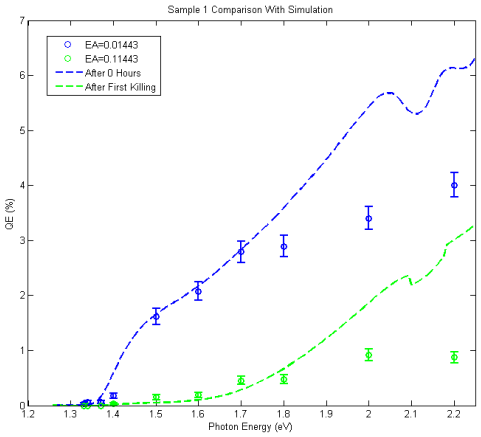

Fig. 12.— Selected spectral response curves and their corresponding Monte Carlo simulations.