A MONTE CARLO PHOTOCURRENT/PHOTOMISSION COMPUTER PROGRAM

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Abstract

A Monte Carlo computer program (POEM) has been developed for the computation of photocurrents and photoemission in gamma (x-ray)-irradiated materials. The program has been used for application to the computation of radiation-induced surface currents on space vehicles and the computation of radiation-induced space-charge environments (IEMP) within space vehicles. The program has been successfully correlated with published expirmental data.

POEM is a composite analytical-Monte Carlo computer program which calculates the photoemission from a gamma (x-ray)-irradiated slab of material. The program uses analytical routines to calculate photon flux attenuation, energy deposition and electron production within the slab, and uses a Monte Carlo routine to calculate the electron transport through the slab and the emission from the slab. The objective of using the analytical photon transport routine is to avoid the computation time-consuming complexity of a pure Monte Carlo model. When using a Monte Carlo photon transport routine, in order to produce a sufficient number of Compton scattering and photoelectric interactions to afford reasonable statistics for the initial energy-angle distributions of the electrons requires a great number of photon histories (typically several hundred thousand histories). To reduce the computation time required, an analytical routine has been incorporated in POEM to compute photon transport.

The POEM program calculates the net photocurrent within a material and the electron emission current from a material including the energy flux, energy spectrum, and angular distribution for an arbitrary incident photon spectrum. The emission can be calculated in either the direction of the incident photon flux or the reverse direction. In either case the program assumes normal incidence of the photon flux on the emitting slab, although with minor modification the program could treat an arbitrary angle of incidence. It is assumed that the time-dependence of the electron emission current is the same as the time-dependence of the incident photon flux, i.e. the model is quasistatic.

The emission calculation includes the Compton electrons, photoelectrons (K and L), and Auger electrons (L) resulting from the scattering and absorption of the primary x-ray flux. The emission calculation, at present, does not include second generation (knock-on) electrons nor the electrons produced by the scattering and absorption of fluorescent or bremsstrahlung radiation. A study is planned to investigate techniques for the inclusion of these effects, including a more rigorous treatment of the Compton scatter radiation.

I. Introduction

The description of the current density and energy-angle distribution of gamma ray or x-ray induced electron emission is required in the study of transient radiation effects on electrical systems and in the development of fast radiation detectors. A rigorous calculation of the electron emission requires both a Monte Carlo photon transport calculation of the electron source distributed throughout the irradiated matter and a Monte Carlo electron transport calculation of the intensity and energy-angle distribution of the multiple scattered electron flux at the emission surface. Because of the low quantum efficiency for the production of primary electrons (Compton, Auger, and photoelectrons) by photons, it has been experienced that a very large number of photon histories are required in the Monte Carlo photon transport calculation to produce a statistically acceptable description of the electron source. Several hundred thousand photon histories have been found necessary for a typical incident photon environment, requiring on the order of 40 minutes computation time (using the ONE-D [1] code on the GE 635 computer). The need exists for a less costly computational tool. A purely analytical electron emission model [2, 3], on the other hand, while providing an inexpensive computation of the electron emission flux, does not properly treat electron multiple scattering and so does not provide a valid description of the angular distribution of emission.

The POEM (photoemission) computer program was developed to provide a computational tool for the calculation of photon radiation-induced electron emission which would be relatively inexpensive to use but would include a proper treatment of electron multiple scattering. POEM is a composite analytical-Monte Carlo program, using analytical routines to calculate photon flux attenuation and primary electron production in the material and a Monte Carlo routine to calculate the electron transport to the surface of the material. Whereas a typical electron emission calculation required 45 minutes computation time (on the GE 635) with a pure Monte Carlo code, the same calculation requires only 3 minutes computation time with POEM, without apparent, significant sacrifice in accurancy.

POEM calculates the electron emission from a gamma or x-ray irradiated slab of material. The program assumes normal incidence of the x-ray flux on the emitting slab, although with minor modification the program could treat an arbitrary angle of incidence. The emission current, energy spectrum, and angular distribution are calculated both in the direction of the incident radiation and in the reverse direction. (Hence,

the program may be used to calculate the net primary photocurrent across any plane within the irradiated material.) It is assumed that the time-dependence of the electron emission current is the same as the time-dependence of the incident photon flux, i. e. the model is quasistatic.

The emission calculation includes the Compton electrons, photoelectrons (K and L), and Auger electrons (L) resulting from the scattering and absorption of the primary x-ray flux and (in an approximate treatment) the Compton scattered x-ray flux. The emission calculation, at present, does not include second generation (knock-on) electrons nor the electrons produced by the scattering and absorption of fluorescent or bremsstrahlung radiation. The electron transport calculation is strictly valid only for electron energies greater than the K absorption edge of the emitting material. The code seems to produce reasonable results, however, down to somewhat lower energies.

POEM has been evaluated through the comparison of computational results to published experimental data for electron emission induced by CuK_α x-radiation and Co^{60} gamma radiation, and through comparison to superflash x-ray-induced electron emission data obtained by the author. The comparisons to the published data are presented herein.

II. Program Description

II.1 Photon Transport

The radiation intensity I (photons/cm^2) at the point x of initiation of electron emission is calculated assuming a simple exponential attenuation of the intensity,

$$I (x, E_\gamma) = I_0 (E_\gamma) e^{-\mu x} \tag{1}$$

where $I_0 (E_\gamma)$ is the incident intensity, x is the distance from the irradiated surface, and μ is the total linear attenuation coefficient. The assumption of exponential attenuation, of course, implies the complete absorption of a photon in any interaction. This is strictly true only of the photoelectric interaction. In a Compton scatter interaction, the photon recedes from the point of collision with reduced energy and altered direction. This Compton scattered radiation is treated by an approximation: rather than reducing the photon flux by decreasing the energy of each Compton scattered photon while holding the number of photons constant (which would considerably complicate the calculation), the number of photons is reduced in each Compton interaction holding the photon energy constant. Mathematically this is done by introducing a Compton attenuation cross-section σ' which is the sum of the Compton absorption cross-section σ_α and a fraction f of the Compton scatter cross-section σ_s,

$$\sigma' = \sigma_\alpha + f \sigma_s \tag{2}$$

The total linear attenuation coefficient μ is then given by

$$\frac{\mu}{\rho} = \tau + \sigma_\alpha + f \sigma_s \tag{3}$$

where τ is the photoelectric cross-section and ρ is the density. Values for the fudge factor f have been selected by comparisons of exponential attenuation calculations to Monte Carlo calculations.

II.2 Electron Production

The irradiated slab is divided into incremental slabs of thicknesses Δx such that $\mu \Delta x << 1$, i. e. so that the photon flux variation through the zone is calculated in each zone for which there is a significant probability of escape, i. e. in each zone for which the maximum path length of the electrons produced in the zone is larger than the normal distance to the emitting surface. (Remember that the maximum electron path length is considerably greater than the extrapolated electron range range because of multiple scattering.)

The number of Compton electrons produced (per cm^2) in a zone, location x_i, by photons of energy E_γ is

$$N_c (E_\gamma, x_i) = I (E_\gamma, x_i) (1 - e^{-\frac{\sigma}{\rho} \Delta x})$$

where $\sigma = \sigma_\alpha + \sigma_s$ is the total Compton mass attenuation coefficient and the photon intensity I (E_γ, x_i) is given by equation [1]. The initial energy-angle probability distributions of the Compton electrons are given by Klein-Nishina. [4]

The number of photoelectrons produced in the zone x by photons of energy E_γ is

$$N_\rho (E_\gamma, x_i) = I (E_\gamma, x_i) (1 - e^{-\frac{\tau}{\rho} \Delta x})$$

where τ is the photoelectric mass attenuation coefficient. It is assumed that for all photon energies greater than the K edge the ratio of L to K photoelectrons produced is equal to the ratio at just above the K edge, i. e.

$$\frac{n_L}{n_K} = \frac{\tau (E_K - \epsilon)}{\tau(E_K + \epsilon) - \tau (E_K - \epsilon)} \tag{6}$$

where E_K is the K edge and ϵ is an infinitesimal energy increment. The angular distribution of the photoelectrons is given by Fischer and Sauter (4), the former for low energy photelectrons ($\beta << 1$), the latter for high energy electrons ($\beta \simeq 1$).

The number of Auger electrons (L only) produced in the zone x_i by photons of energy E_γ is

$$N_A (E_\gamma, X_i) = (1 - f_K) N_\rho^K (E_\gamma, x_i) \tag{7}$$

where N_p^K is the number of K photoelectrons produced and f_K is the K fluorescence yield given by.[5]

$$f_K \cong \frac{z^4}{z^4 + 30^4} \qquad (8)$$

where Z is the atomic number. The angular distribution of the Auger electrons is assumed isotropic.

The total electron initial energy-angle probability distribution for each zone of the emitter is calculated by summing for each photon energy the Compton, photoelectric and Auger distributions and then integrating over the photon energy spectrum.

II.3 Electron Transport

The transport of the electrons to the emitting surface is calculated using the POET [6] Monte Carlo electron transport program which has been incorporated into POEM. POET is a condensed history Monte Carlo program. In the condensed history Monte Carlo method, the results of multiple scattering theory are combined with Monte Carlo techniques to form a consistent approach to electron transport calculations in the media of finite dimensions. Since the large majority of electron-atom interactions involve small angel deflections and small energy loss, the condensed history random walk approach is applicable to electron transport (it is not applicable to photon transport due to the large scattering angles involved in the majority of collisions). Rather than calculate the trajectories of the electrons as they undergo each coulomb interaction, a random walk computation is performed in such a way that each step takes into account the combined effect of many collisions. The electron history is divided into logarithmically-spaced energy intervals. For each step of the random walk the path length increment traveled by the electron, corresponding to the energy loss increment, is computed using the Bethe-Moller stopping power. [7-9] By random sampling from the angular distributions calculated using the Goudsmitt-Saunderson theory [10] of multiple scatter, the direction of travel of the electron after each random walk step is obtained.

For each electron history the random walk computation is initiated by random selection of an initial location within the electron production zone (from a uniform distribution within the zone) and a random selection of the initial electron energy and velocity direction (from the computed energy-angle probability distribution for the zone). The random walk computation is continued until either the electron escapes from the emitting surface or until the residual path length of the electron is smaller than the normal distance to the distance to the emitting surface (so that in this continuous slowing down approximation the electron has zero probability of escape).

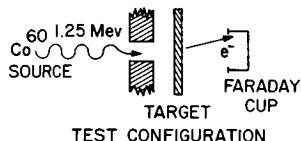## III. Comparison of Computational Results With Experiment Data

III.1 Energy Spectrum

E. P. Denisov, et. al [11] of Leningrad State University published in 1963 the results of an expirment in which the structures of the x-ray photoemission energy spectra from aluminum, titanium, chromium, and iron photocathodes were measured. The photocathodes consisted of a thin layer of the test material (thicker than the maximum exit depth of the electrons) sputtered on a planar glass substratum at the center of an evacuated, spherical collector. The energy structure of the photoemission was determined by measuring the collected current as a function of the bias potential between the photocathode and the collector. The photocathodes were irradiated by CuK_α x-rays (8 kev). The experimental results for the four photocathodes are compared to the POEM calculations of the energy structure shown in Figure 1. The experimental and calculational results are compared by adjusting the arbitrary normalizations such that the primary maxima are equal. (No attempt was made to compare the gross emission currents since these data were not published by Denisov, et. al.). The agreement of the structures of the calculated and the experimental spectra is good except for the low energy spike in the experimental spectrum, which Denisov, et.al. interpret to be the secondary electron contribution to the emission spectrum. The three peaks in the energy spectrum due to the K photoelectron, L photoelectron, and Auger electron contributions to the spectrum can be seen in both the calculated and measured spectra.

III.2 Emission Current, Angular Distribution

Ebert and Lauzon [3] of the Lawerence Radiation Laboratory published in 1965 the results of an experiment in which they measured the quantum efficiency (electrons emitted per incident photon) and the angular distribution of the gamma-ray induced electron emission from carbon, aluminum, copper, cadmium, and lead targets. Two sets of target thicknesses were used: one set of targets with thickness equal to the range of a 1.25 MeV photoelectron, and another set with thickness of one-tenth the range. The targets were irradiated by a collimated beam of 1.25 MeV gammas from a Co^{60} source. The emission current was measured by a Faraday cup; the (cumulative) angular distribution was measured by varying the solid angle subtended by the Faraday cup.

The Ebert and Lauzon results are compared to the POEM calculations for the quantum efficiency in Table 1 and for the (differential) angular distribution shown in Figure 2. The agreement in both quantum efficiency and angular distribution is excellent. The agreement in quantum efficiency is not remarkable; Ebert and Lauzon had comparable success using an analytical model to calculate quantum efficiency. What is significant is the

TEST CONFIGURATION

TARGET	THICKNESS (CM)	POEM	EXPERIMENT
CARBON	2.03×10^{-1}	9.68×10^{-3}	9.14×10^{-3}
	2.26×10^{-2}	2.57×10^{-3}	2.46×10^{-3}
ALUMINUM	2.27×10^{-1}	7.96×10^{-3}	7.97×10^{-3}
	1.27×10^{-2}	1.80×10^{-3}	1.99×10^{-3}
COPPER	5.24×10^{-2}	6.10×10^{-3}	6.13×10^{-3}
	5.12×10^{-3}	2.09×10^{-3}	2.04×10^{-3}

QUANTUM EFFICIENCY (ELECTRON/PHOTON)

TABLE 1. COMPARISON OF POEM RESULTS WITH EXPERIMENTAL DATA OF EBERT AND LAUZON [3]

agreement in the angular distribution. Ebert and Lauzon found that calculations of the angular distribution made using an analytical model, which assumed rectilinear electron transport, were in complete disagreement with the experimental data. Here, then, is the key advantage .of the Monte Carlo calculation: analytical models which cannot properly treat electron multiple scattering, but rather assume rectilinear transport, provide no valid information as to the angular distribution of photoemission.

Conclusions

Comparisons of computational results with experimental data have shown the POEM code to be quite adequate for the calculation of photon radiation-induced electron emission, at least in the limited ranges of photon energies for which test data were available for comparison. More test data, especially in the x-ray energy range, 1 keV to 1 MeV, are required for additional code verification. One shortcoming of the POEM code is its neglect of the secondary (knock-on) electrons. A study is planned of computational techniques for the inclusion of the secondary electrons in the emission calculation.

References

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(11) E. P. Denisov, V. N. Schemelev, A. N. Mezhevich, and M. A. Rumsh, "Analysis of the Energy Structure of X-Ray Photoemission From a Massive Cathode, "Soviet Physics, Solid State 6, (1965) p. 1047.
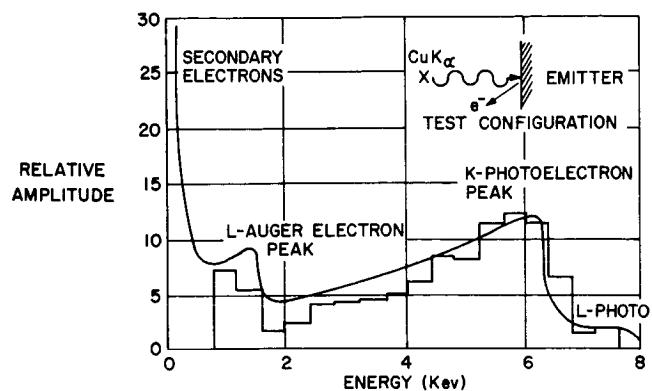
Figure 1a. Electron Emission Energy Spectrum –
Aluminum --- Comparison of Calculations with
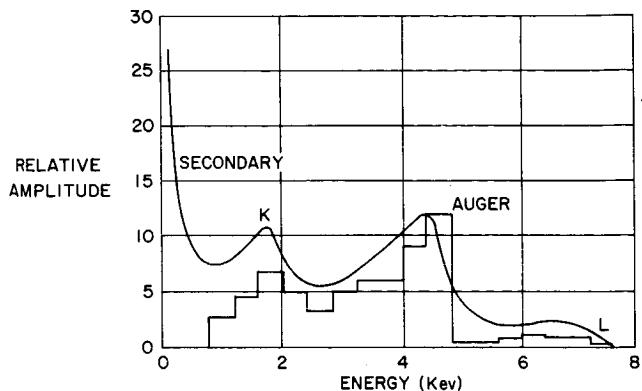Experimental Data (CuK α x-Radiation
Incident on Target)

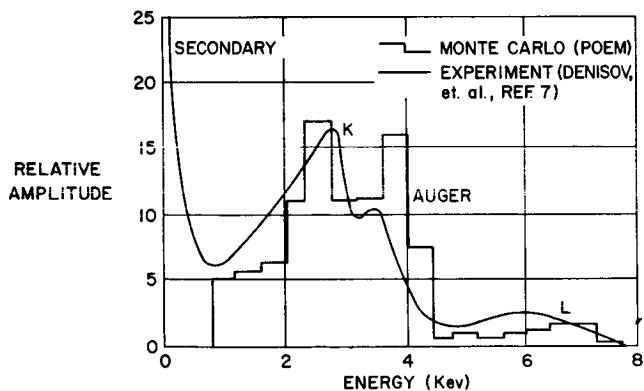**Figure 1c.** Electron Emission Energy
Spectrum – Chromium

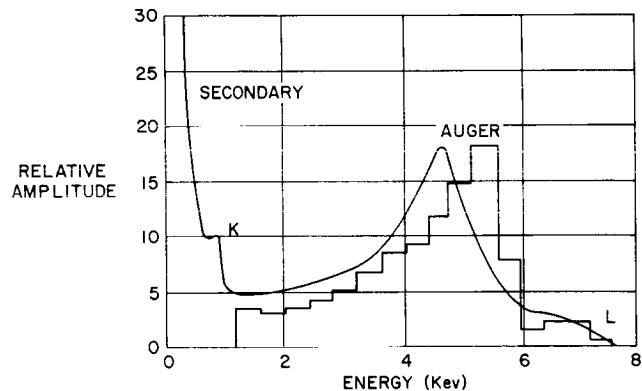**Figure 1b.** Electron Emission Energy
Spectrum – Titanium

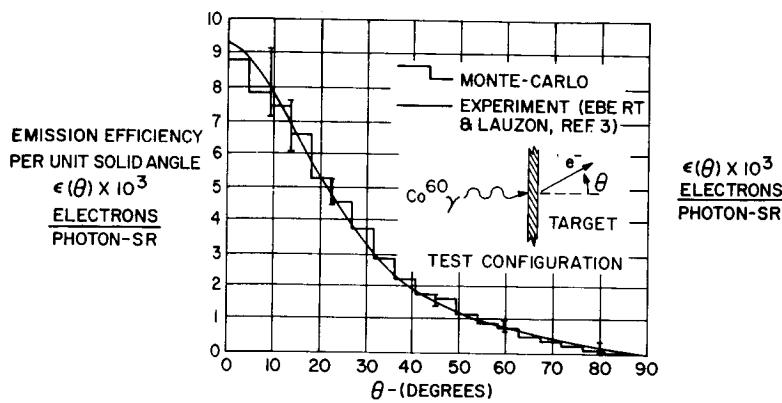**Figure 1d.** Electron Emission Energy
Spectrum – Iron

Figure 2a. Electron Emission Angular Distribution –
Carbon Target (Electrons Per Unit Solid Angle
Per Incident Photon) (1.25 Mev Co^{60} Gamma
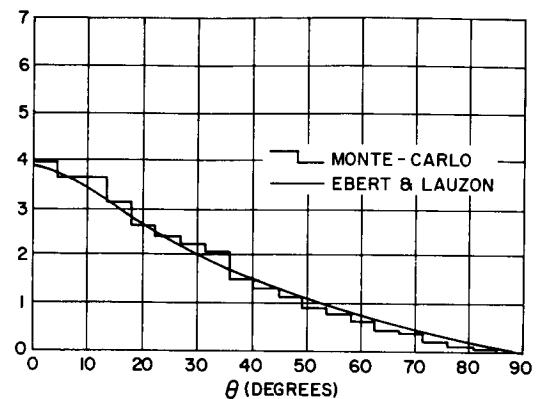Radiation on Target)

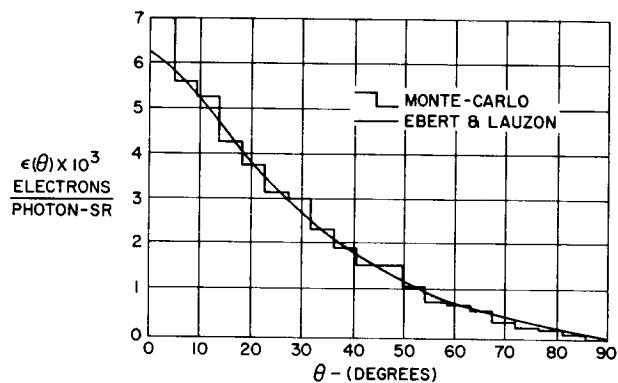Figure 2c. Electron Emission Angular
Distribution – Cooper Target

Figure 2b. Electron Emission Angular
Distribution – Carbon Target