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TITLE: INCORPORATION OF MONTE CARLO ELECTRON INTERFACE STUDIES INTO PHOTON GENERAL CAVITY THEORY

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INCORPORATION OF MONTE CARLO ELECTRON INTERFACE STUDIES INTO PHOTON GENERAL CAVITY THEORY

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Electron Monte Carlo calculations using CYLTRAN and a new PHSECE (Photon Produced Secondary Electrons) technique were carried out to estimate electron fluences and energy deposition profiles near LiF/Al and LiF/Pb material interfaces undergoing Co-60 gamma irradiation. Several interesting and new features emerge: (i) Although the build-up of the secondary electron fluences at the interfaces of the irradiated media is approximately exponential, the value of the electron mass fluence build-up coefficient, β_B , is not equal to the electron mass fluence attenuation coefficient, β_A . (ii) The attenuation of the gamma-generated electron fluences at the cavity-medium interfaces, β_A, is strongly dependent on the Z of the adjacent material, and (iii) for LiF/Pb there is a significant "intrusion" energy deposition mode arising from "side-scattering" in the wall (Pb) material.

These new features of interface dosimetry [at least (i) and (ii)] are incorporated into the photon general cavity expressions of Burlin-Horowitz and Kearsley and compared with experimental data.

I. Introduction - Photon General Cavity Theory

Photon general cavity theory has recently been reviewed by Horowitz[1]. The Burlin photon general cavity expression[2]

$$f_{cm} = d\,\bar{S}_{cm} + (1 - d)\,\overline{(\mu_{en}/\rho)}_{cm} \qquad (1)$$

its modification by Horowitz[3]

$$f = \frac{(Z/A)_c}{(Z/A)_m}\left\{1 + d\left[\frac{(Z/A)_m}{(Z/A)_c}\,S_{cm} - 1\right] + d'\left[\frac{(\mu_{en}/\rho)_c}{(\mu_{en}/\rho)_m}\,\frac{(Z/A)_m}{(Z/A)_c} - 1\right]\right\} \qquad (2)$$

and a new approach incorporating electron backscattering at the cavity-medium interfaces[4]

$$f_{cm} = d_1\,\bar{S}_{cm} + d_2\,\overline{(\mu_{en}/\rho)}_{cm} \qquad (3)$$

was compared to the landmark Co-60 photon experimental study by Ogunleye at al[5] of LiF-TLDs embedded in media of polystyrene, aluminum, copper and lead. In the Burlin expression d is given by

$$\int_0^g \exp(-\beta x)dx \Big/ \int_0^g dx = \frac{1 - \exp(-\beta g)}{\beta g} = d \qquad (4)$$

where g is the average path-length of electrons crossing the cavity and β is the electron mass fluence attenuation coefficient. The Burlin-Horowitz expression incorporates the fact that, in general, the average path-length for radiation crossing the cavity, g, need not equal the average path-length for radiation created within the cavity, g', as assumed by Burlin and many other investigators. d' is then the volume average of the build-up of the electron fluence generated by photon interactions within the cavity and is not equal to 1-d. Although it has been convenient to assume that the build-up of electrons is exponential and governed by the same mass attenuation coefficient as the attenuation coefficient of the medium spectrum within the cavity, the Monte Carlo calculations reported on herein clearly indicate the contrary (See Figures 1 and 2).

The constraint $d+d' = 1$ incorporated into the Burlin expression is thus clearly violated not only by the non-equality of g and g' but also by the non-equality of the attenuation coefficients governing the attenuation of the medium spectrum within the cavity and the build-up of the cavity-generated electron spectrum within the cavity.

In the Kearsley expression, the factors d_1 and d_2 are given by

$$d_1 = (1 - b_w)(\lambda_1(w, c)) \tag{5}$$

and

$$d_2 = 1 + (\lambda_1(w, c))b_w(1 - b_c)(1 - e^{-\gamma t}) - (\lambda_1(c, c))(1 - b_c)[1 + b_c(1 - e^{-\gamma t})]. \tag{6}$$

A full description of the mathematical formulation is given elsewhere[1,4]; b_w and $b_c(t)$ are backscatter coefficients defined as the probability that an electron crossing an interface will cross it again; t is the thickness of the cavity, $< \lambda_1(w,c) >$ is a propagation factor describing the attenuation and backscattering properties of the electron energy fluence within the cavity and γ is a factor describing the exponential build-up of the cavity-generated electron fluence. The Kearsley expression has the familiar Burlin form of the effective stopping power except, of course, that $d_1 + d_2 \neq 1$ in agreement with the Burlin-Horowitz expression.

In common with all three expressions is a required knowledge of both β and g (the Kearsley expression requires, in addition, knowledge of backscatter coefficients) and the choice of the value of these parameters has been the subject of considerble confusion and uncertainty in the literature on the applications of photon general cavity theory.

Due to the lack of experimental or theoretically derived values of β for Compton and/or photoelectric effect-generated electron fluences, the usual approach has been to adopt values of β derived from the attenuation of β-ray spectra, (which are based on a one-to-one correspondence between E_{max} and β), even though it is well known that the exponential attenuation of β-ray spectra is an accidental consequence of the shape of β-ray spectra and of the differences between the scattering and absorption of electrons that have various initial energies.

β was measured for beta rays in LiF by Paliwal and Almond[6] with the result

$$\beta_{LiF} = 14/E_{max}^{1.09} \quad \text{for } 0.23 \text{ MeV} < E_{max} < 2.27 \text{ MeV} \tag{7}$$

whereas for higher energy monoenergetic electrons between 8 and 20 MeV

$$\beta_{LiF} = 37.9/E_{max}^{1.61} \tag{8}$$

leading to $\beta = 13.4\ cm^2g^{-1}$ for Co-60 generated secondary electron spectra, and this value has indeed been used by many investigators in the analysis of LiF cavity data. An analysis and review[1] of the application of all three photon general cavity expressions to the experimental data of Ogunleye et al[5] lead to the following general conclusions:

(i) For LiF in polystyrene and Al the general trend of the results is to decreasing values of χ^2/n with increasing β and at $\beta = 13.4\ cm^2g^{-1}$ all three expressions were in satisfactory agreement with experiment ($\chi^2/n \leq 1$).
(ii) For the case of severly mismatched cavity and medium (i.e., LiF in Pb), the three expressions yielded minimum χ^2/n at different values of β ; 15 cm^2/g, 18 cm^2/g and 6 cm^2/g for the Burlin, Burlin-Horowitz and Kearsley expressions respectively.

II. Electron Monte Carlo Calculations

The work described herein reports on the results of electron Monte Carlo calculations specifically designed to resolve this apparent discrepancy and uses the coupled, cylindrically symmetric, electron-photon Monte Carlo code CYLTRAN[7] with a new production biasing scheme. A mono-directional beam of Co-60 photons is perpendicularly incident on various thicknesses of LiF embedded in media of aluminum and lead in semi-infinite plane geometry in order to accurately simulate the experiments of Ogunleye et al who used LiF spacers to eliminate edge effects. Electron and photon collisions are individually tracked, and the electron-photon fluences and dose distributions are separately recorded as they penetrate the wall and cavity media.

Production and transport of photon/electron cascades to .001 MeV are treated in detail. Electron interactions include elastic/inelastic nuclear scattering, inelastic atomic electron scattering, and the corresponding generation of secondary photons (e.g., fluorescence and bremsstrahlung). Photons, in turn, generate pair, Compton, and photoelectrons; multishell relaxations can occur as a result of electron impact and photoionization events. The relaxation model yields Auger electrons and characteristic x-rays appropriate to the excited state of the atom undergoing transition to the ground state. Annihilation quanta are also produced and transported. Electron cross-sections used are those compiled in the DATPAC4[8] library; whereas, the Biggs-Lighthill[9] library is used for photon cross-sections.

Monte Carlo estimation of highly space-resolved electron fluences and energy deposition near material interfaces presents a particularly difficult problem. Deposition profiles near material boundaries are typically steep requiring ultra-thin geometrical zone structure to resolve the profile slope.

Often, photons easily traverse such thin zones without interaction, thereby undersampling the secondary electron production within that zone. In principle, running sufficiently more histories solves this problem; however, run time and cost become prohibitive. In order to obtain sufficiently accurate secondary electron production in ultra-thin zones one must bias the natural game of sampling secondary electron sources. Conventional photon interaction biasing schemes, such as forcing collisions within specific zones, frequently generate unacceptable variance fluctuations. When there exists numerous ultra-thin zones, these fluctuations are amplified. The PHSECE (Photon Produced Secondary Electrons) technique was developed to alleviate this difficulty.

Essentially, PHSECE allows biased electron production along any arbitrarily small photon path-length, independent of the occurrence of an explicit photon interaction. Therefore, if a photon traverses any given zone without interaction, the correct number (and energy) of secondary electrons along that path-length is sampled. This is accomplished by integrating (using Monte Carlo) the appropriate production cross-section over that path-length. Russian roulette is also used in conjunction with PHSECE to keep the secondary electron population manageable. PHSECE is considered to be in the developmental stages and future improvements will yield even more efficiency for simulating this type of interface problem.

III. Results

Several interesting and new features of interface dosimetry emerge (See Figures 1 and 2):

(i) Although the buildup of the LiF cavity-generated secondary electron fluence is indeed approximately exponential, as assumed in the development of the Burlin expression and in previous application of photon general cavity theory, the value of the exponential build-up coefficient $\beta_B = 5.48 \pm 0.13$ cm^2g^{-1} (curve c) is not equal to the mass attenuation coefficients discussed below and is certainly far removed from $\beta = 13.4$ cm^2g^{-1}.

(ii) The attenuation of the gamma-generated electron fluences at the cavity medium interfaces, although again approximately exponential in nature, is dependent on the Z of the adjacent "up-stream" material, introducing an additional heretofore unexpected complication into the theoretical treatment of photon cavity effects. Neglecting the non-exponential behavior of the attenuation at large penetration depths we obtain $\beta_A = 6.67 \pm 0.17 cm^2g^{-1}$ for Co-60 generated electron fluences in LiF crossing the Pb/LiF interface (curve b) and $\beta_A = 7.46 \pm 0.14$ cm^2g^{-1} (curve g) for electrons crossing the Al/LiF interface.

It is further interesting to note that only for the Pb/LiF/Pb configuration is there a significant difference between the electron fluence mass attenuation coefficient and the energy fluence mass attenuation coefficient, the latter increasing to 8.32 ± 0.25 cm^2g^{-1}. These values of β_A are in strikingly improved agreement with the predictions of the Kearsley fit to the Ogunleye et al data and serve as strong experimental confirmation of the

Kearsley expression. The variability of β_A for Co-60 generated secondary electron fluence is further illustrated by the attenuation data in Al and Pb,

β_A = 9.98 ± 0.15 cm^2g^{-1} in Al crossing a LiF interface (curve i)

β_A = 16.9 ± 0.28 cm^2g^{-1} in Pb crossing a LiF interface (curve e)

(iii) For severely mismatched cavity-medium interfaces, e.g., LiF in Pb, there is a significant "intrusion" energy deposition mode arising from "side multiple scattering" in the wall (Pb) material (curve d in Fig. 2). It should be noted that this process is distinct from electron backscattering at the LiF/Pb interface (S_2) and which is reflected in the increase of the electron flux distribution (curve c) at S_2.

IV. Implications to Photon General Cavity Theory

We believe we have demonstrated unequivocally that the constraint d+d'=1 in the Burlin expression is unphysical due both to the lack of equality between g and g' (established by Horowitz et al[1,3] and the lack of equality between β_A and β_B (demonstrated herein). The previously reported good agreement between the predictions of the Burlin expression and experiment[5] (using β =13.4 cm^2g^{-1}) for LiF in Al and polystyrene was coincidental and due to a fortuitous cancellation of errors. Figure 3 shows values of χ^2/n plotted versus g/t for LiF in Al for all three cavity expressions using β_A =7.46 cm^2g^{-1} and β_B =5.48 cm^2g^{-1} for the B-H and Kearsley theories. For the Burlin expression the constraint d+d'=1 forces $\beta_A = \beta_B$ =7.47 cm^2g^{-1}. At g/t = 1.58 (obtained from $g = \int_0^{\pi/2} t\,\frac{P(\theta)d\theta}{\cos\theta}$ averaged over a typical collimated Co-60 gamma spectrum and $P(\theta)$ is the

Klein-Nishina electron angular probability distribution function for gamma ray Compton scattering - see reference 1 for a discussion concerning uncertainties in the estimation of g) the Burlin expression now yields a marginally satisfactory $\chi^2/n = 2.2$. Taking into account the reduction of the electron fluence from its equilibrium value in Al to its value crossing the front Al/LiF interface (curve f) yields $\chi^2/n = 1.1$ for the Burlin-Horowitz expression at $g/t = 1.58$ and using $g' = g/2$. The B-H expression thus seems to have maintained its validity for moderately mismatched cases of LiF cavity and medium which gives it a practical advantage over the Kearsley expression due to its far greater simplicity. f_k is calculated in Fig. 3 using an arbitrarily chosen value of $\alpha = \beta_\beta$. Further calculations are in progress to determine the behaviour of f_k with α for both the Pb/LiF/Pb and Al/LiF/Al configurations.

For LiF in Pb the results shown in Fig. 4 indicate a minimum value of chi-squared equal to 0.4 for the Kearsley expression at $g/t = 1.1$. The trend towards decreasing g/t for optimal results in the Pb/LiF/Pb configuration compared to $g/t = 1.58$ for pure Compton scattering is reasonable due to the strong, more forward-scattered photoelectric component in Pb $\left((\sigma/\rho)/(\sigma/\rho)' \cong 0.3 \text{ at } 1.25 \text{ MeV}\right)$. The results thus clearly support the Kearsley expression, its prediction of greatly reduced values of β_A compared to the predictions of expression[7] and its treatment of the electron transport problem for strongly mis-matched cavity-medium configurations where significant electron backscattering and "intrusion" dose deposition mechanisms are operative. More work is required to understand the behavior of β_A, specifically its dependence on gamma ray energy and the Z of the adjacent wall material. In addition, accurate application of the Kearsley expression requires knowledge of $b_e(t)$, the exponential backscatter coefficient, as yet unknown.

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Figure Captions:

Figure 1 - Electron flux distribution as a function of material thickness for the Al/LiF/Al configuration. Curve f shows the build-up of the electron flux in Al as a function of penetration depth and curve g shows the attenuation of the Al generated electron flux as a function of penetration depth in LiF. The non-exponential behavior at large penetration depths does not significantly affect the cavity theory calculations.

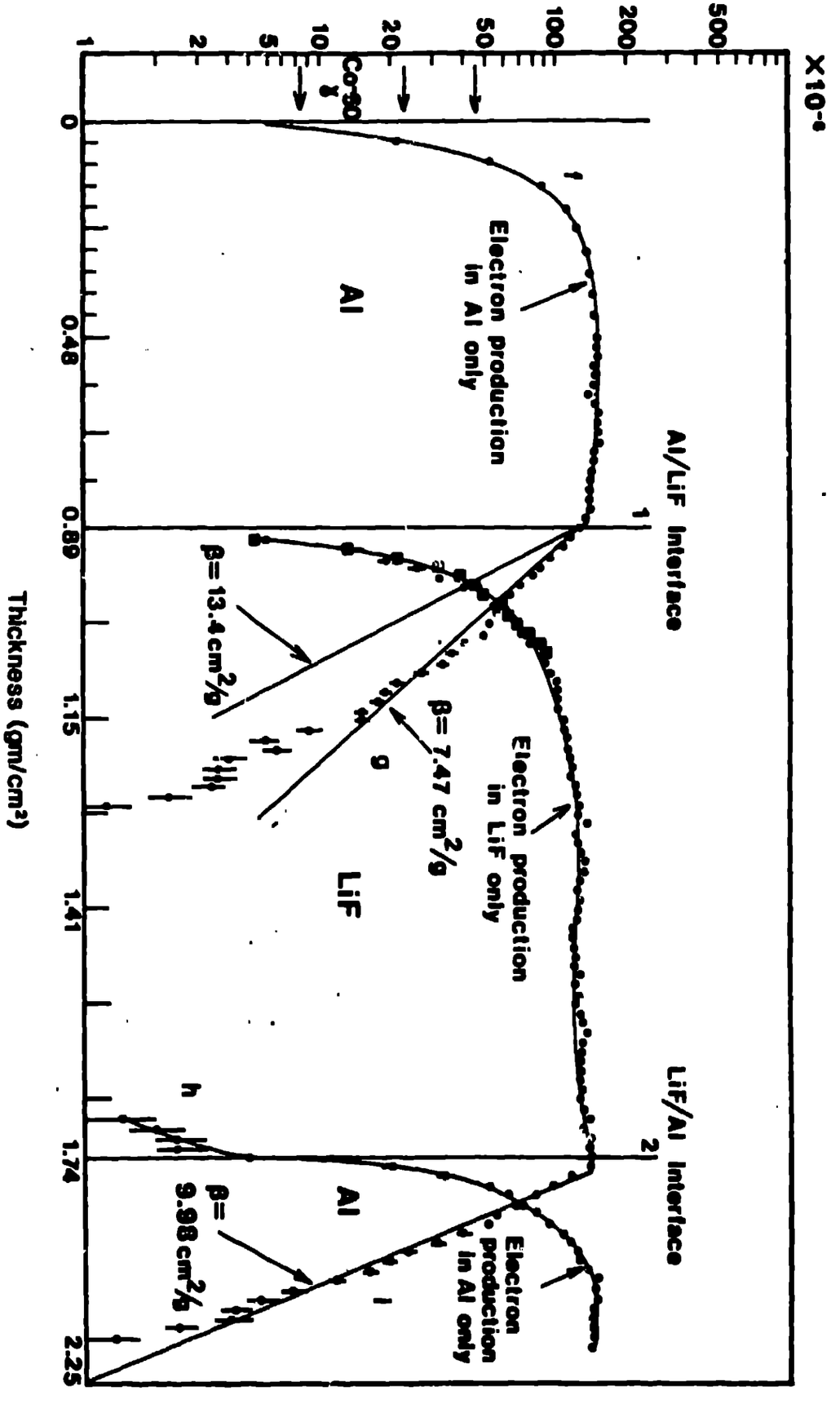
Figure 2 - Electron flux distribution as a function of material thickness for the Pb/LiF/Pb configuration. Curve C shows the build-up of the electron flux in LiF as a function of penetration depth (°LiF only, ▫Pb/LiF, gamma interactions in LiF only). The slight difference between the two curves does not significantly affect the cavity theory calculations. Note the significant reduction in the electron flux in Pb as one approaches the Pb/LiF interface.

Figure 3 - Values of chi-squared as a function of g/t for the Al/LiF/Al configuration using the experimental data of Ogunleye et al[5]. Over the range of physically realistic values of g/t, $1.0 \leq g/t \leq 2.0$, the Burlin-Horowitz expressions yields significantly superior agreement with experiment.

Figure 4 - Values of chi-squared as a function of g/t for the Pb/LiF/Pb configuration using the experimental data of Ogunleye at al[5]. Values of f_k were calculated assuming an arbitrarily chosen value of $\alpha = 5.48\ cm^2g^{-1}$.

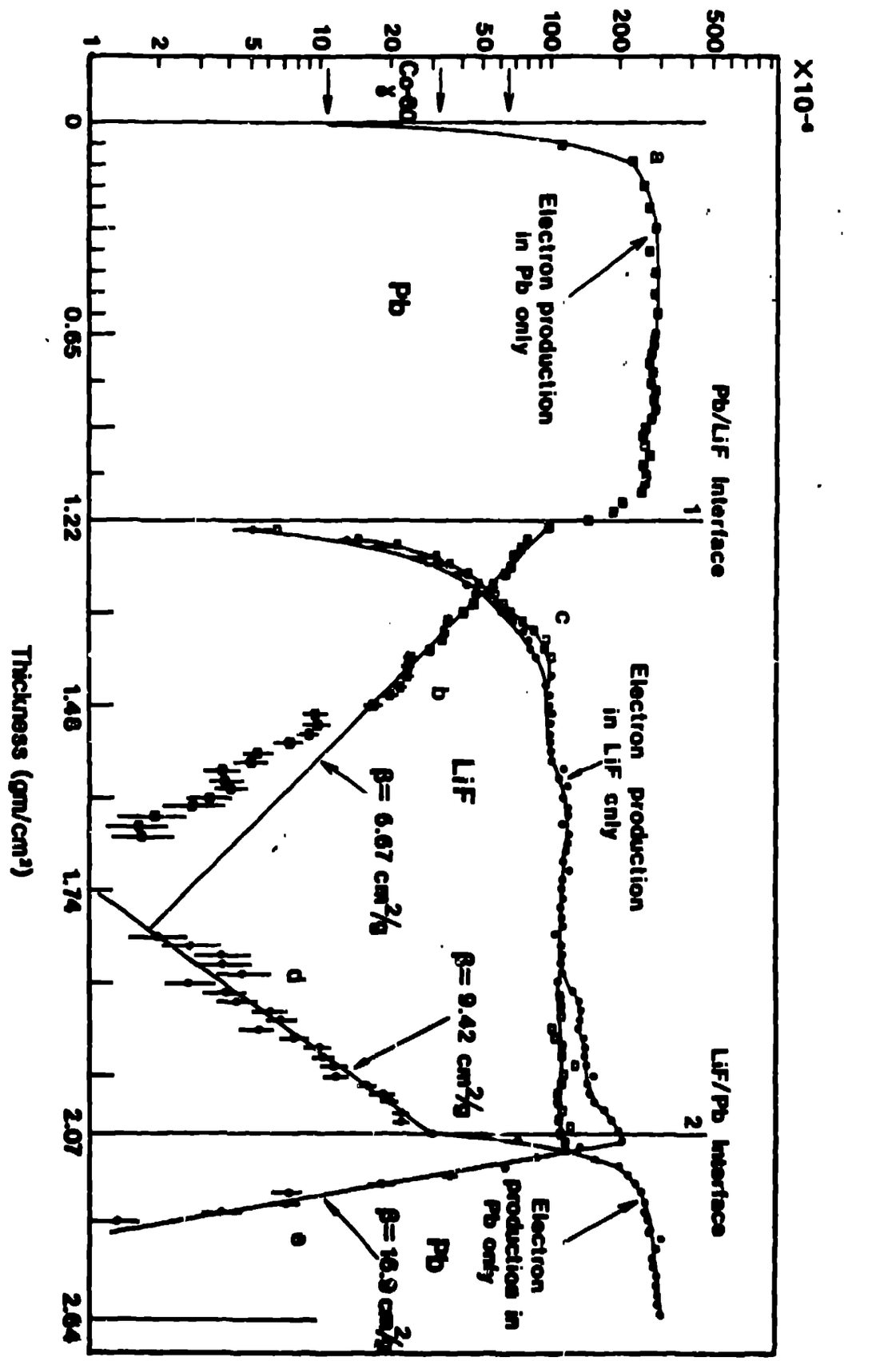
ELECTRON FLUX DISTRIBUTION

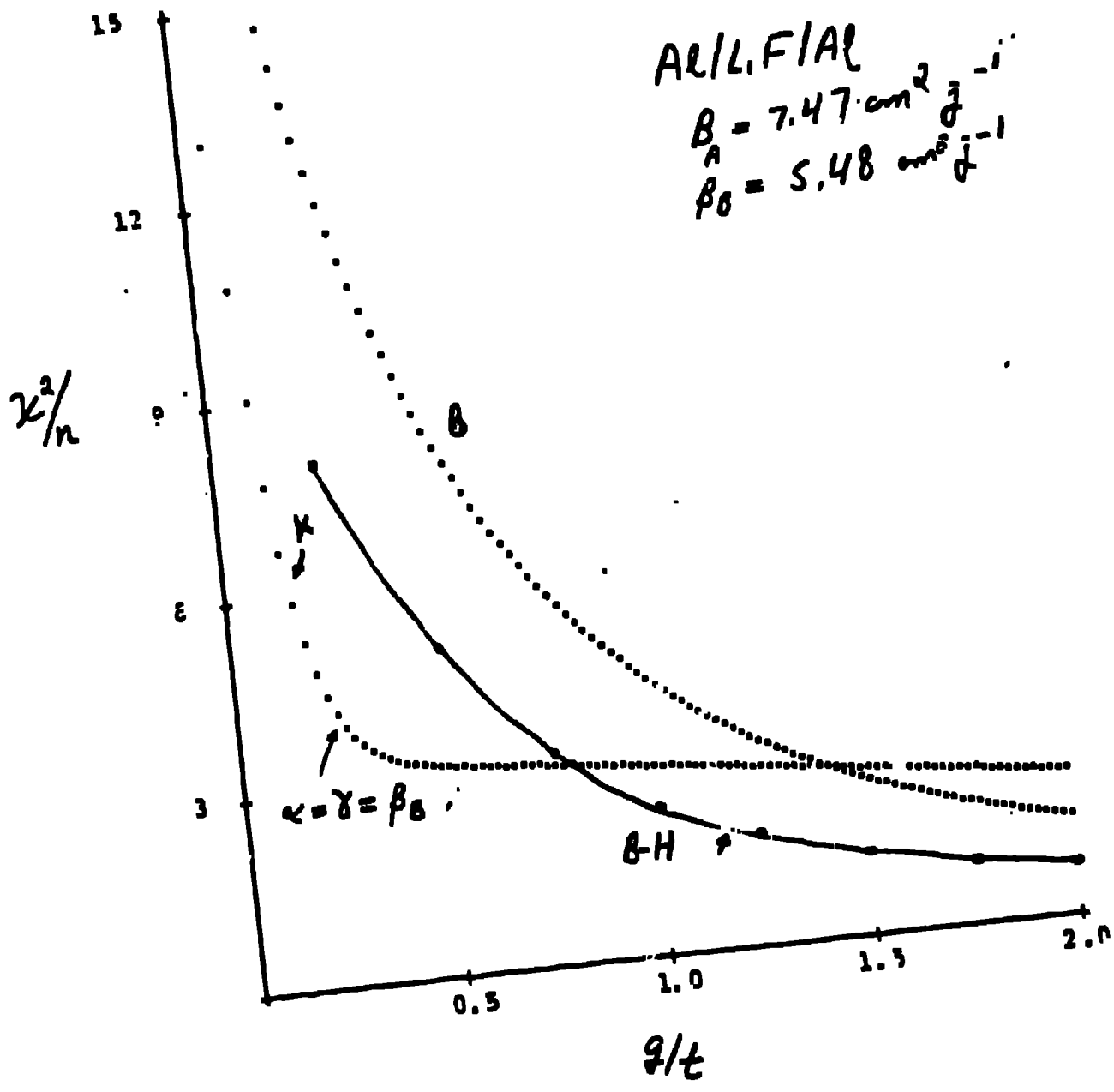
(TRACK-LENGTH / VOLUME-MEV, NORMALIZED TO ONE INCIDENT PARTICLE)



ELECTRON FLUX DISTRIBUTION

(TRACK-LENGTH / VOLUME-MEV, NORMALZED TO ONE INCIDENT PARTICLE)

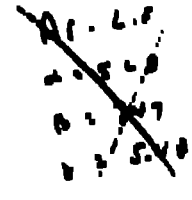


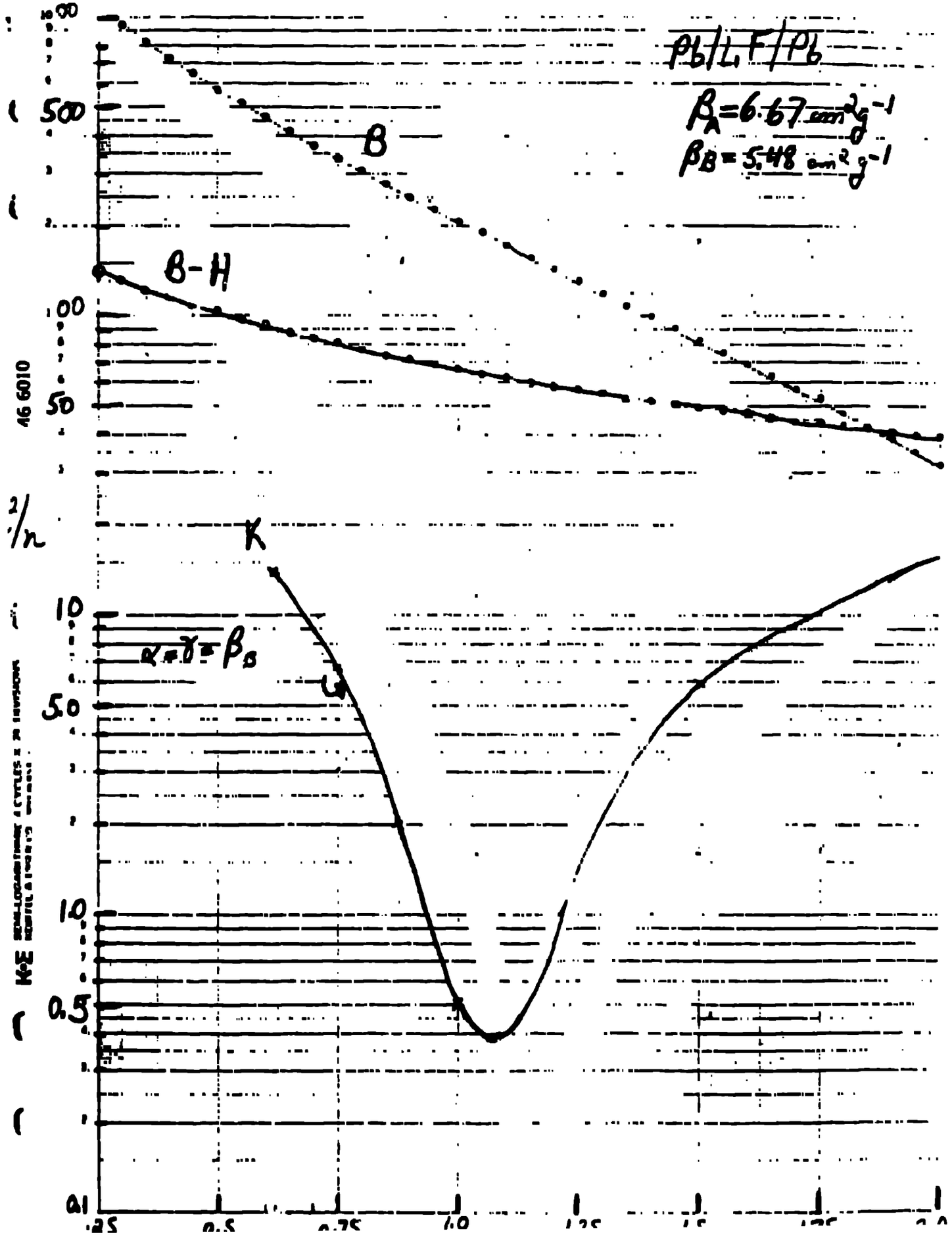


AL/L.F/AL

$B_A = 7.47 \cdot cm^2 \cdot g^{-1}$

$\beta_B = 5.48\ cm^2\ g^{-1}$




Pb/LiF/Pb
$\beta_\lambda = 6.67\ cm^2 g^{-1}$
$\beta_B = 5.48\ cm^2 g^{-1}$
B
B-H
K
$\alpha = \gamma = \beta_B$
500
100
50
10
5.0
1.0
0.5
0.1
2/n
46 6010
.25
0.5
0.75
1.0