Study of the Electron-Positron Annihilation Coincidence Peak Two-Dimensional Profile

E. do Nascimento, O. Helene, V. R. Vanin,

Instituto de Física, Universidade de São Paulo, C.P. 66318, 05389-970, São Paulo, SP, Brazil

and C. Takiya

Departamento de Ciências Exatas, Universidade Estadual do Sudoeste da Bahia, Vitória da Conquista, BA, Brazil

Received on 20 October, 2003

Positron annihilation radiation profile in aluminum was observed with a pair of Ge detectors in coincidence. ^{22}Na was used as a source of positron and the two-dimensional gamma energy spectrum was fitted using a model function. Annihilation components of positron at rest with conduction band, 1s, 2s, and 2p electrons were observed. The in-flight positron annihilation was also observed. The model function also took into account the detector response function, relative efficiency corrections and the gamma backscattering. Coincidences involving a combination of Compton effect, pileup, ballistic deficit, and pulse shaping problems were treated as well.

1 Introduction

This study aimed to understand the shape of the electron-positron annihilation peak measured in coincidence by two photon detectors (Fig. 1).

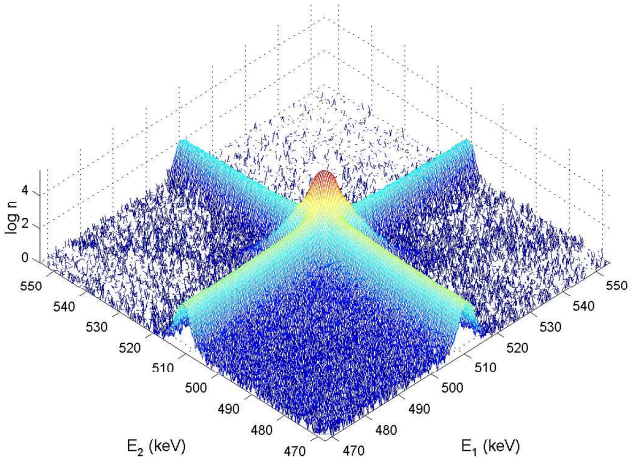

Figure 1. Distribution of coincident events as a function of the measured energies E_1 and E_2, showing the Doppler broadening.

The proper fit of the 511 keV-511 keV peak requires many analytical functions, giving information about the electron momentum distribution in the analyzed material. This technique is known as Coincidence Doppler Broadening (CDB) of the electron-positron annihilation radiation [1]and is used in studies of the electronic and atomic strutures of defects in solids [2, 3, 4].

2 Experimental Setup

The profile of the annihilation peak of positrons from a ^{22}Na source in metallic Al was measured with the Linear Accelerator Laboratory residual radioactivity multi-detector array (MULTI) [5]. The two annihilation gamma-rays were measured with a pair of Ge detectors in coincidence, placed in diametrically opposed positions, separated by 15 cm, and with a 3.7×10^5 Bq (10 μCi) ^{22}Na source. This source was placed between two 2 mm thick aluminum sheets (99.999% pure). An ^{192}Ir source was simultaneously measured to provide references for detector calibration and follow any energy calibration drift during the experiment. The measurement run lasted for 200 h, when 1.5×10^7 events in the peak region were accumulated.

3 Model Function

Usually the results of Doppler broadening measurement are analyzed comparing the calculated annihilation probability density with the experimental data. In this work we opted for another procedure. The convolution of the detector response function with empirical functions to represent the gamma-rays emitted after positron annihilation with 1s, 2s, 2p and conduction electrons were calculated. All these functions were parametrized. This procedure avoids the dificult problem of deconvolution of the Doppler broadening spectrum [6] .

The function model was determined from a qualitative analysis of the experimental data and published theoretical results [7, 8]. Positron annihilation with band electrons was fitted by three arcs of parabola and one gaussian along the

line $E_1 + E_2 = 1022$ keV:

$$f_b = \sum_{i=1}^{3} C_i(E_1 - E_2 - \alpha_i)(E_1 - E_2 + \alpha_i) + \frac{A_b e^{\frac{-(E_1-E_2)^2}{2\sigma_b^2}}}{\sqrt{2\pi}\sigma_b}$$

where E_1 and E_2 are energies in detectors 1 and 2 respectively, and α_i are the cutoff parameters ($C_i = 0$ when $|E_1 - E_2| > \alpha_i$). Positron annihilation with 1s electrons was fitted by one gaussian along the line $E_1 + E_2 + B_{1s} = 1022$ keV:

$$f_{1s} = \frac{A_{1s} e^{\frac{-(E_1-E_2)^2}{2\sigma_{1s}^2}}}{\sqrt{2\pi}\sigma_{1s}}$$

where B_{1s} is the binding energy of the 1s electrons. Positron annihilattion with 2s electrons was fitted by two gaussians along the line $E_1 + E_2 + B_{2s} = 1022$ keV:

$$f_{2s} = \frac{A_{2s} e^{\frac{-(E_1-E_2)^2}{2\sigma_{2s}^2}}}{\sqrt{2\pi}\sigma_{2s}} + \frac{A'_{2s} e^{\frac{-(E_1-E_2)^2}{2\sigma'^2_{2s}}}}{\sqrt{2\pi}\sigma'_{2s}}$$

where B_{2s} is the binding energy of the 2s electrons. Positron annihilation with 2p electrons was fitted by one gaussian along the line $E_1 + E_2 + B_{2p} = 1022$ keV:

$$f_{2p} = \frac{A_{2p} e^{\frac{-(E_1-E_2)^2}{2\sigma_{2p}^2}}}{\sqrt{2\pi}\sigma_{2p}}$$

where B_{2p} is the 2p electron binding energy. Finally, in-flight positron annihilation was fitted by:

$$f_f = \frac{A_f e^{-\lambda d} e^{\frac{-(E_1-E_2)^2}{2\sigma_f^2}}}{\sqrt{2\pi}\sigma_f}$$

where

$$d = \frac{m_0 c^2}{\sqrt{2}} - \sqrt{(E_1 - \frac{3m_0c^2}{2})^2 + (E_2 - \frac{3m_0c^2}{2})^2}$$

(Fig. 2). The $A's$ and σ's are the areas and widths of the gaussians respectively. Detection effects due to ballistic deficit, pile-up and Compton scattering (Fig. 3) were considered in the fit. Coincidences involving a combination of Compton effect, pileup, ballistic deficit, and pulse shaping problems (Fig. 4), backscatering (Fig. 5) and efficiency corrections of the detectors in the fitting region, were taken into account. The model functions were fitted to the experimental data and the result is shown in Fig. 6.

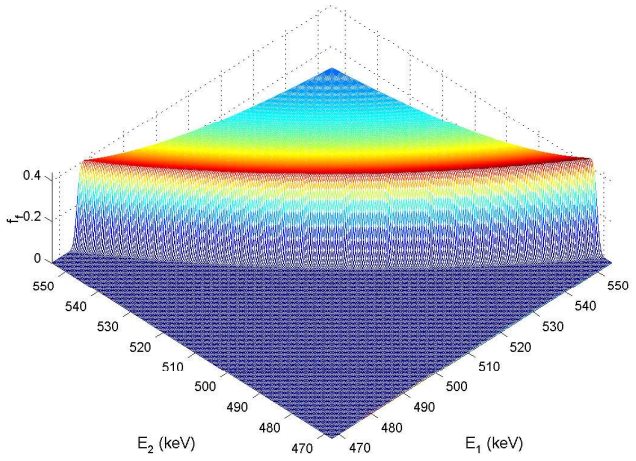

Figure 2. Two-dimensional representations of in-flight positron annihilation radiation.

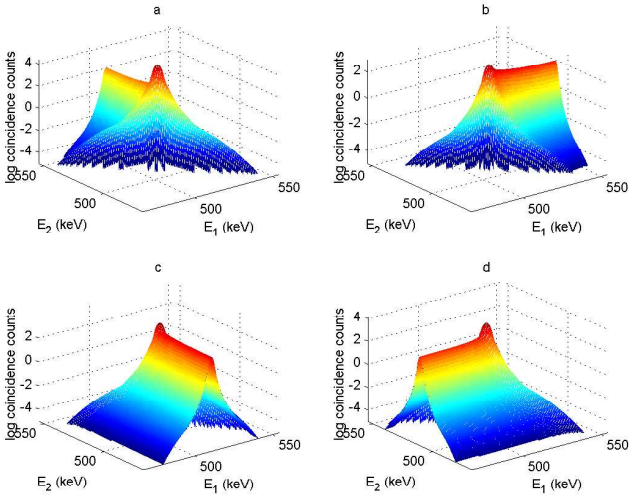

Figure 3. Two-dimensional representations of the fitted exponential tails of the electron-positron annihilation peak. The internal exponentials tails for detectors 1 and 2 are represented in parts (a) and (b) respectively. The external exponential tails for detectors 1 and 2 are in (c) and (d), respectively.

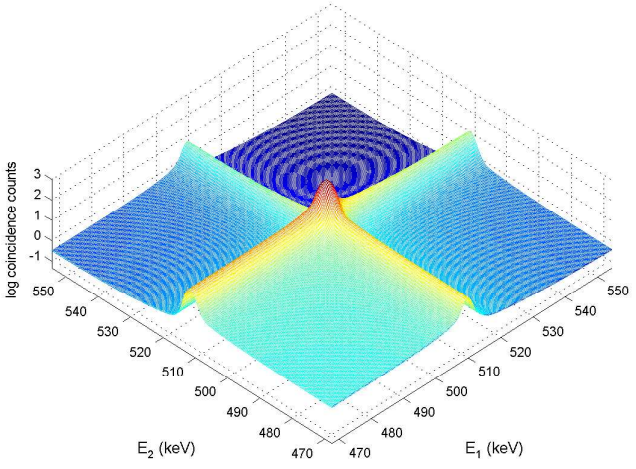

Figure 4. Two-dimensional representations of Compton-Compton and other effects.

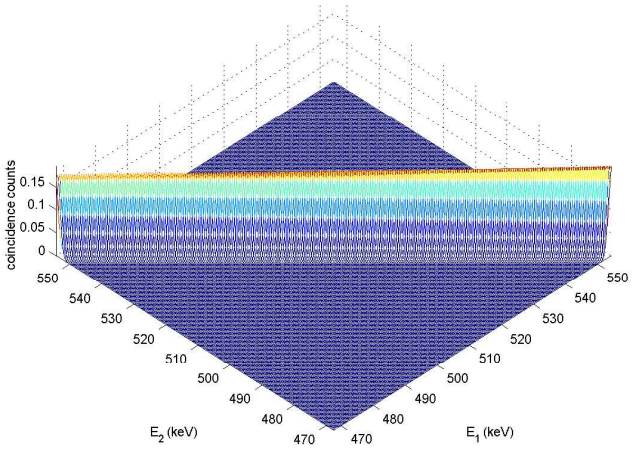

Figure 5. Two-dimensional representations of the backscattering coincidence.

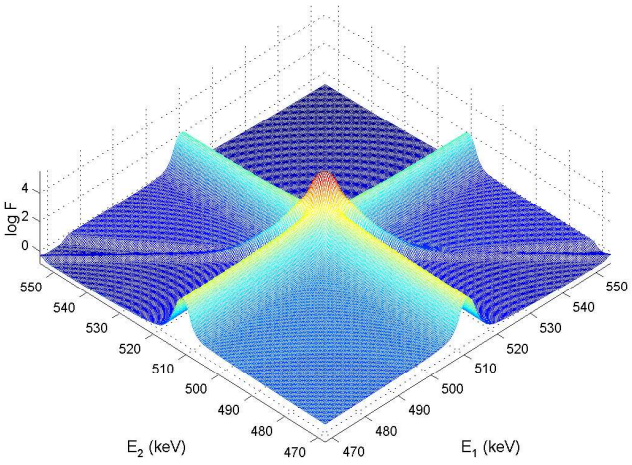

Figure 6. The fitted coincidence spectrum.

The fit was done by the least-squeares method (see, for instance [9]) with the Gauss-Marquardt algorithm due to the non-linearity in the parameters [10]. The chi-squared value was calculated by

$$\chi^2 = \sum_{i,j} \frac{(n_{ij} - F_{ij})^2}{F_{ij}}$$

where n_{ij} is the number of observed events in channel (i, j) of the coincidence spectrum (Fig. 1), and F_{ij} is the fitted function (Fig. 6).

4 Conclusion

The reduced χ^2 obtained in this study, 1.1 with about 62448 degrees of freedom, does not show a disagreement between the data and the model, suggesting that a complete statistical analysis of the coincidence Doppler broadening annihilation radiation is possible. Better model functions can be considered in order to improve the χ^2 value [1].

Acknowledgments

We wish to acknowledge the support of Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq, Fundação de Amparo à Pesquisa do Estado de São Paulo - FAPESP, and the Data Section of the International Atomic Energy Agency.

References

[1] P. E. Mijnarends, A. C. Kruseman, A. van Veen, H. Schut, and A. Bansil, J. Phys. Condens. Mat. **10**(46) 10383 (1998).

[2] M. Hasegawa, Z. Tang, Y. Nagai, T. Nonaka, and K. Nakamura, Appl. Surf. Sci. **194**, 76 (2002).

[3] Y. Nagai, Z. Tang, H. Ohkubo, K. Takadate, and M. Hasegawa, Rad. Phys. Chem. **68**, 381 (2003).

[4] M. J. Puska and R. M. Nieminen, Rev. Mod. Phys. **66**, 841 (1994).

[5] V. R. Vanin, R C Neves, et. al., XIX Reunião de Trabalho sobre Física Nuclear no Brasil (1996)

[6] C. Takiya, O. Helene, E. do Nascimento, V. R. Vanin, Nucl Instr Meth A (2004) in press.

[7] Z. Tang, M. Hasegawa, Y. Nagai, M. Saito, and Y. Kawazoe, Phys. Rev. B **65**, 045 108 (2002).

[8] V. J. Ghosh, M. Alatalo, P. Asoka-Kumar, B. Nielsen, K. G. Lynn, A. C. Kruseman, and P. E. Mijnarends, Phys. Rev. B **61**, 10 092 (2000).

[9] V. R. Vanin, G. Kenchian, M. Moralles, O. A. M. Helene, and P. R. Pascholati, Nucl. Instr. Meth. A **391**, 338 (1997).

[10] D. W. Marquardt, J. Soc. Appll. Math. **11**, 431 (1963).