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Novel data evaluation algorithm for Coincident Doppler Broadening Spectroscopy

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ABSTRACT

In Coincident Doppler Broadening Spectroscopy (CDBS) the sum energy of the annihilation photons is checked to be 1022 keV, to validate the measurement of an undisturbed two-gamma electron–positron decay event. The events are stored in a two-dimensional acquisition matrix. A new algorithm is presented, which optimizes the extraction of the one-dimensional CDBS spectrum from this matrix by enhanced background suppression by the use of variable size bins.

1. Introduction

Coincident Doppler Broadening Spectroscopy (CDBS) is widely used to characterize element-vacancy complexes [1], precipitates [2] or embedded thin layers [3]. Its advantage over single-detector Doppler Broadening Spectroscopy (DBS) is its ability to analyze the chemical environment of the positron annihilation site. This requires a signal to noise ratio (SNR) of the recorded γ-spectrum better than 10^5 to measure annihilations with strongly bound core electrons [4]. The low background is achieved by the evaluation of the sum energy of the annihilation photons resulting from the electron positron pair. It is regarded to be $\hat{E} = 2 \cdot m_0c^2 = 1022$ keV in the case of the valid detection of a two-γ electron–positron-decay in collinearly arranged detectors [4,5].

Because of charge collection times in semiconductor detectors, the acquisition rate of a detector pair in coincidence should not exceed ≈ 1000 counts/s to ensure reliable coincidence identification. The low core annihilation rates down to 10^{-3} [6] result in necessary acquisition times for CDBS measurements performed with a single pair of detectors of several hours or more. For this reason, it is necessary to perform the background suppression as accurately as possible, and to evaluate the valid events with the highest efficiency. In this paper, first the types of measurement disturbances, which lead to the background, are described and then a new algorithm for effective evaluation of the measured data is presented.

2. CDB spectra composition

The Doppler shifted energy of the positron annihilation radiation can be measured in both γ-photons of the dominant $2-\gamma$ decay. One ideal detector would be sufficient for the complete acquisition of the Doppler broadened annihilation line. An ideal spectrum of the annihilation radiation is schematically shown in Fig. 1.

The best available detectors for the energy resolved analysis of the annihilation radiation are High purity Germanium (HPGe) detectors. HPGe detector measurements may be affected by several different distortions intrinsic to the technology:

1. The detectors have a typical energy resolution of about 1.3 keV at 511 keV γ-energy. This leads to a convolution of the γ-spectrum with an approximately Gaussian resolution function.
2. γ–photon interaction with the detector occurs in two possible ways for 511 keV-photons: Either by photo effect or by Compton effect. The photo effect deposits the total energy of the photon in the detector (Fig. 2, areas d and e), whereas Compton scattering leads to a continuous spectrum from 0 keV to E_C=340 keV. (The Compton edge corresponds to the highest energy, which is deposited by Compton scattering in the detector crystal, see Fig. 2, area a.) E_C is sufficiently far away from the Doppler broadened 511 keV line so that Compton scattering does not directly influence Doppler broadening spectroscopy.
3. Compton scattering outside of the active detector volume: In particular, γ–photons are scattered between the source and the detector and the detector measures a lower γ-energy (Fig. 2, area b). Because the energy loss $\Delta E_\gamma = \cos \Phi * E_C$ is low for a small scattering angle, it cannot be distinguished if a photon

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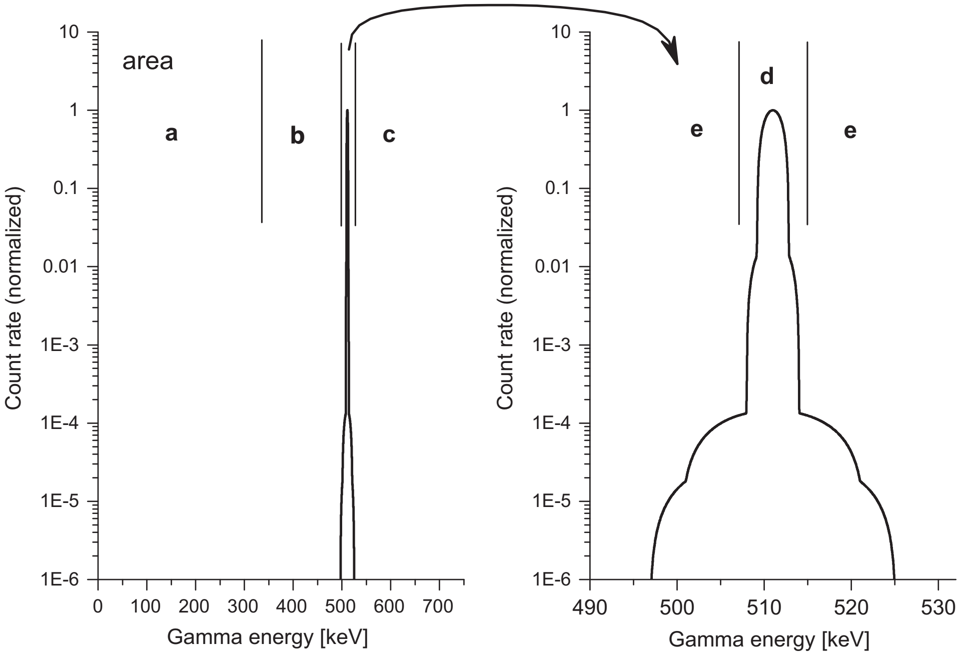

Fig. 1. The schematic spectrum of the positron annihilation line. Area (e) contains the high momentum Doppler shifts, which are most interesting for the analysis of annihilations with core-electrons. (The plots in Figs. 1 and 2 are schematic. Levels of high-momentum Doppler broadening, noise and Compton scattering are comparable to experimental results.)

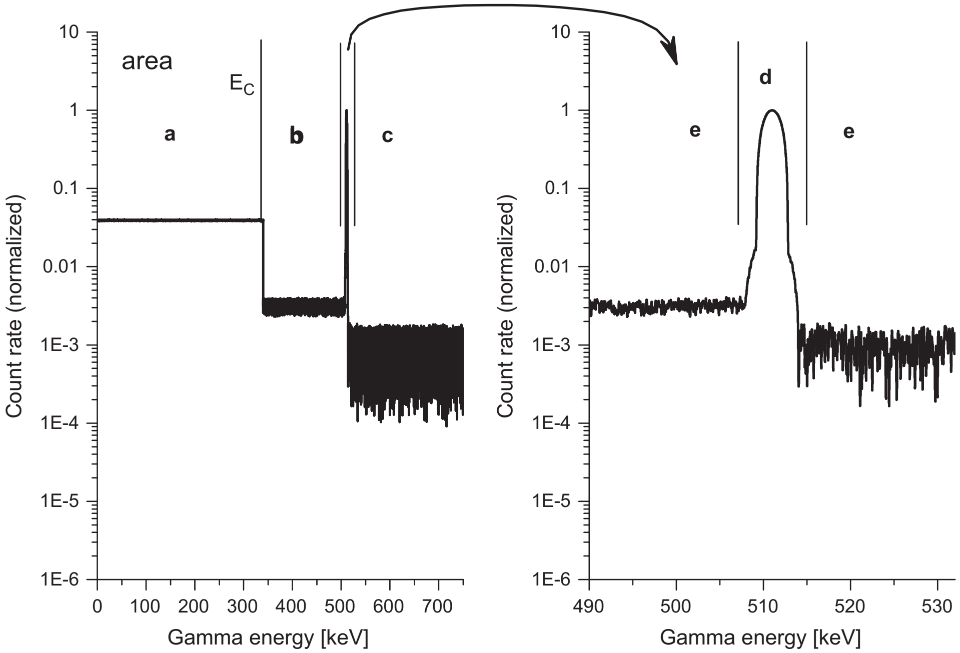

Fig. 2. Gamma ray detection is disturbed by several effects (see text). Area (e) of the Doppler broadened annihilation peak is hidden by the background. Compare with Fig. 1.

slightly below 511 keV is Doppler-shifted or small-angle scattered. This generates a significant background in the low energy side of the annihilation line.

4. The $3-\gamma$ decay of ortho-positronium, which can always be formed when positrons reach surfaces, has also a continuous contribution to areas a and b.
5. Incomplete charge collection in the detector crystal also contributes mainly to area b.
6. Pile-up: The stochastic time distribution of the emitted positrons allows two decays to occur in the same time interval not resolved by the signal acquisition, so that the detector measures the sum of both deposited energies. Because most pile-up events are affected by Compton scattering, an additional background is produced over the whole energy region which is of importance for Doppler broadening spectroscopy (Fig. 2, areas a–c).
7. Positron reflection: Even if all positrons are ideally focused onto the sample, some of them get reflected and annihilate at some other part of the spectrometer. A single detector cannot distinguish their radiation from annihilations in the sample.

These effects decrease the SNR of single detector measurements to about 10^3. As it can be seen in Fig. 2 this does not allow to reveal