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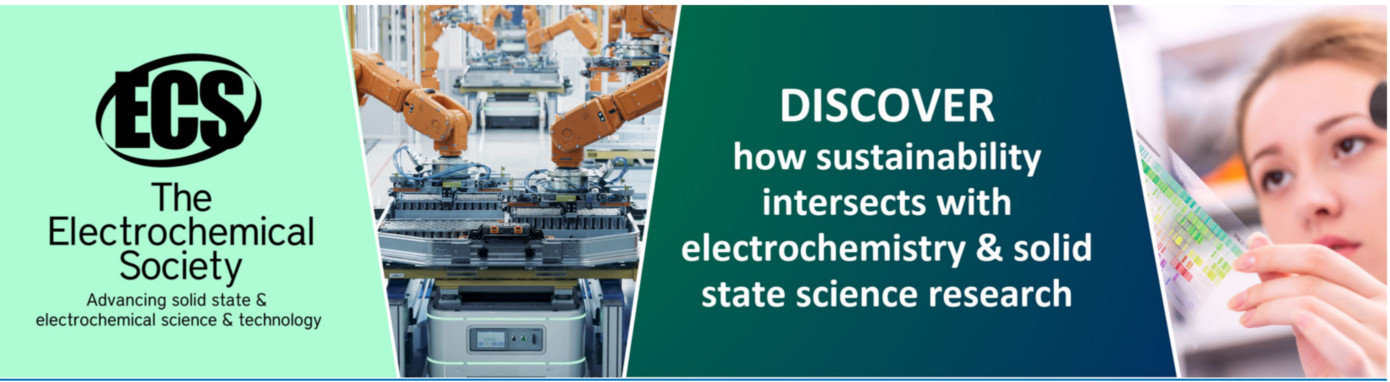

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Determination of electron binding energies in two-dimensional Coincident Doppler Broadening spectra

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Abstract.
In Coincident Doppler Broadening Spectroscopy (CDBS) the 1022 keV sum energy of the annihilation photons is utilized to validate an undisturbed detection of the two-gamma electron-positron decay. Due to conservation of energy the sum energy is lowered if the annihilating particles, in particular the electron, are in a bound state. Usually this effect is neglected because the binding energies of annihilated electrons are small compared to the energy of the annihilation photons. A novel data evaluation algorithm allows to clearly identify the influence of binding energies in the CDBS spectrum. Exemplary measurements are presented and compared to calculated spectra.

1. Introduction

As described in widely known publications [1–3] the low background of coincident Doppler broadening measurements is based on the evaluation of the sum energy $\hat{E}$ of an annihilating electron positron pair. It is regarded to be $\hat{E} = 2 \cdot m_0c^2 = 1022\,\mathrm{keV}$ in the case of the detection of a two-γ electron-positron-decay in two collinear detectors. However, the sum energy is not exactly 1022 keV, it is reduced by the binding energies of the annihilating particles E_B. While the binding energy of the diffusing positron is only a few eV [4], the binding energy of core electrons ranges up to many keV. Within the scope of this work, $\hat{E}$ is precisely evaluated in the CDBS spectra and the influences of the binding energy are analyzed.

2. Data evaluation

E_1 and E_2 are the energies of a collinearly emitted photon pair, which are both recorded in a two-dimensional multi-channel-analyzer (MCA) matrix. ΔE designates the Doppler shift of both annihilation, which is representing the longitudinal movement of the electron-positron pair:

$$\hat{E} = E_1 + E_2 = 2 \cdot m_0 c - E_\mathrm{B} = 1022\,\mathrm{keV} - E_\mathrm{B} \quad \Delta E = \frac{E_1 - E_2}{2} \tag{1}$$

Figure 1 illustrates the contributions of different electron orbitals of iron to different areas in the acquisition matrix for ideal data recorded with infinitely high resolution. The Doppler broadening leads to diagonal lines in the spectrum which are limited by the maximal momentum of the electron in the direction of the detector axis. All events on one diagonal line have the

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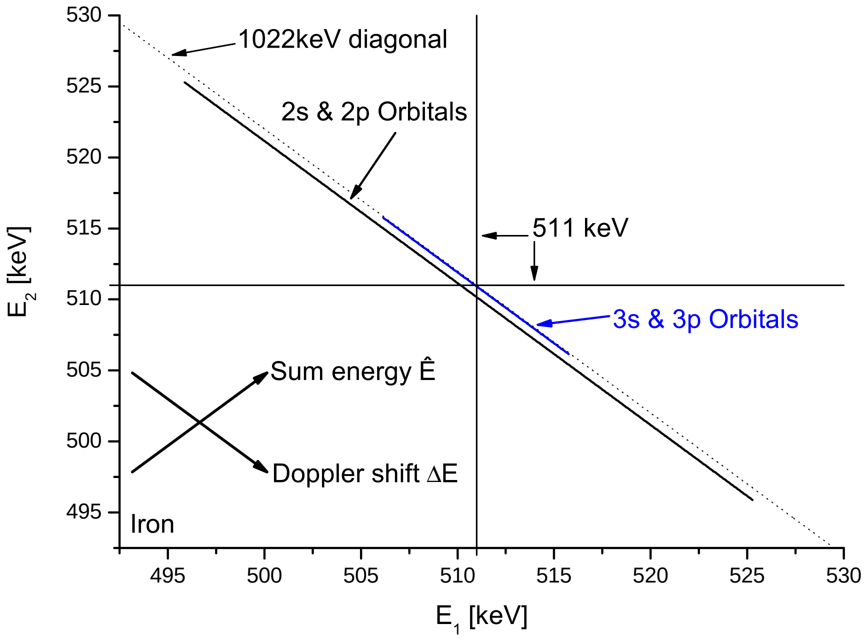

Figure 1. The schematic distribution of annihilation events from different orbitals in the CDB spectrum, exemplarily for iron. The diagonal arrows designate the axis of sum energy and Doppler shift. The distance of an event to the 1022 keV diagonal results from the binding energy E_{B}.

same sum energy according to equation 1. The sum energy varies due to the electron binding energies. With increasing E_B the core annihilation probability P decreases and is negligible for $1s$-electrons (not shown).

In real measurements, these event lines widely overlap because of the finite energy resolution of $\approx 1.3\,\mathrm{keV}$ of HPGe-Detectors [5]. Consequently, the lines of different sum energy are not detected separately, but the variation of the mean sum energy $\hat{E}$ over the Doppler shift ΔE is expected to be observable.

For this task, a novel data evaluation algorithm is used. It determines the mean sum energy $\hat{E}(\Delta E)$ by fitting the Gaussian-shaped detector function to areas in the matrix with constant Doppler shift ΔE. For details about the used algorithms, see [6].

3. Experiment

For the present experiment, annealed iron was chosen as sample material due to its 2s and 2p orbitals, which annihilate with positrons with a probability P of 0.034 % and 0.076 % [7]. The binding energy of these orbitals is 845 eV and 720 eV respectively. In the acquisition matrix, the according events are dominating in the outer wings of the Doppler broadened photo peak - i.e. for $|\Delta E| > 5\,\mathrm{keV}$ - as it is visible in figure 1, whereas the 3p and 3s orbitals practically overlap with the 1022 keV center peak due to their low binding energy of $< 100\,\mathrm{eV}$. Although the annihilation rate with the 2s and 2p orbitals is below 0.1%, the background in the relevant quadrants of the spectrum is in the range of 10^{-5} compared to the photopeak, so that a measuerment of 2p and 2s electron annihilations is feasible. The mean sum energy $\hat{E}$ in the range of high Doppler shifts $|\Delta E| > 5\,\mathrm{keV}$ is expected to be significantly reduced by the electron binding energy.

4. Calculations

For the calculation of the sum energy as a function of the Doppler shift $\hat{E}(\Delta E)$, the contributions from the relevant orbitals are calculated separately. The intensity $I_n(\Delta E)$ of the single orbitals n, which represent one diagonal line in figure 1, is approximated by a parabolic function due to the projection of an isotropic electron momentum distribution to one dimension. The intensity of each line is set to the respective core annihilation probability P_n. $E_{\max,n}$ is the maximal Doppler shift regarding the orbital n.

$$I_n(\Delta E) = \frac{\sqrt{(\Delta E_{\max,n})^2 - (\Delta E)^2}}{\frac{4}{3} \cdot (\Delta E_{\max,n})^3} \cdot P_n \tag{2}$$

The spectra are folded with a Gaussian function with a E_{FWHM} of 1.05 keV which represents the coincident detector resolution $Res(E)$.

$$Res(E) = \frac{1}{\sqrt{\frac{\pi \cdot E_{\mathrm{FWHM}}}{2 \cdot ln2}}} \cdot e^{-\frac{1}{2}\left(\frac{E \cdot 2\sqrt{2ln(2)}}{E_{\mathrm{FWHM}}}\right)^2} \tag{3}$$

$\bar{I}_n(\Delta E)$ is the intensity distribution function of orbital n after convolution with the Gaussian detector function.

$$\bar{I}_n(\Delta E) = (I_n(\Delta E) * Res(E(\Delta E))) \tag{4}$$

The resulting $\hat{E}(\Delta E)$ is the average sum energy of all events as a function of the specific Doppler shift ΔE. n_{max} is the number of orbitals included in the calculation. $E_{\mathrm{B}\,n}$ denotes the binding energy of the respective orbital.

$$\hat{E}(\Delta E) = \frac{\sum_{n=1}^{n_{max}} \bar{I}_n(\Delta E) \cdot (1022keV - E_{\mathrm{B}\,n})}{\sum_{n=1}^{n_{max}} \bar{I}_n(\Delta E)} \tag{5}$$

5. Results

In figure 2 the measured and the calculated sum energy are shown. The statistical error of the measured values is calculated by variance analysis of neighbored but independent evaluation points.

In the momentum area of $15 \cdot 10^{-3} m_0 c < |p| < 30 \cdot 10^{-3} m_0 c$ a significant decrease of $\hat{E}$ is visible. This sum energy deficit is in good agreement with the calculated data. The deviation from the calculated data can be explained by the strongly simplified momentum distribution of the single electron orbitals. For $|p| > 30 \cdot 10^{-3}\, m_0 c$ the measured values scatter largely since the number of events in the evaluated area was to small to detect a stable center of the peak.

6. Conclusion and Outlook

The measurement of the binding energies provides an additional element-specific parameter compared to conventional evaluation of Doppler broadening only. It was shown that the two-γ sum energy as a function of the Doppler shift can be extracted from a two-dimensional CDBS acquisition matrix with a standard event number of $\approx 1.5 \cdot 10^7$ counts. For future applications, this may help interpreting ambiguous CDB results which occur when alloys or elements with a similar CDB-spectrum are measured.

To get more exact $\hat{E}(\Delta E)$-spectra, more experiments with higher statistics and better energy resolution have to be performed. Furthermore material combinations, like iron and cobalt are to be investigated. They carry an almost identical CDBS shape, but may be distinguished by different binding energies.

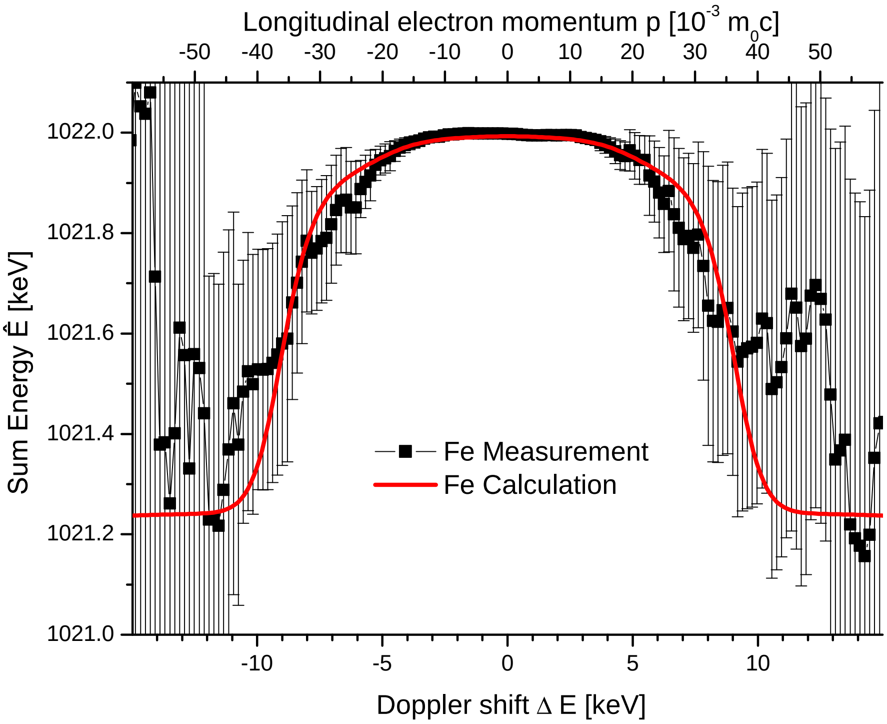

Figure 2. For each Doppler shift ΔE the center of weight $\hat{E}$ of the contributing events is calculated. The sum energy deficit is caused by the binding energy of the annihilated electron.

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