Data Article

Data on pure tin by Positron Annihilation Lifetime Spectroscopy (PALS) acquired with a semi-analog/digital setup using DDRS4PALS

Danny Petschke*, Ricardo Helm, Torsten E.M. Staab

University Wuerzburg, Department of Chemistry and Pharmacy, LCTM Roentgenring 11, D-97070 Wuerzburg, Germany

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A B S T R A C T

Positron annihilation lifetime spectroscopy (PALS) provides a powerful technique for non-destructive microstructure investigations in a broad field of material classes such as metals, semiconductors, polymers or porous glasses. Even though this method is well established for more than five decades, no proper standardization for the used setup configuration and subsequent data processing exists. Eventually, this could lead to an insufficiency of data reproducibility and avoidable deviations.

Here we present experimentally obtained and simulated data of positron lifetime spectra at various statistics measured on pure tin (4N-Sn) by using a semi-analog/digital setup, where the digital section consists of the DRS4 evaluation board, “Design and performance of the 6 GHz waveform digitizing chip DRS4” [1]. The analog section consists of nuclear instrument modules (NIM), which externally trigger the DRS4 evaluation board to reduce the digitization and, thus, increase the acquisition efficiency. For the experimentally obtained lifetime spectra, $^{22}\text{Na}$ sealed in Kapton foil served as a positron source, whereas $^{60}\text{Co}$ was used for the acquisition of the prompt spectrum, i.e. the quasi instrument response function. Both types of measurements were carried out under the same conditions.

All necessary data and information regarding the data acquisition and data reduction are provided to allow reproducibility by other research groups.

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* Corresponding author.
E-mail address: danny.petschke@uni-wuerzburg.de (D. Petschke).

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### Specifications table

| Subject area | Condensed matter physics, materials science, nuclear instrumentation |
|-------------|---------------------------------------------------------------|
| More specific subject area | Positron annihilation lifetime spectroscopy (PALS) on metals |
| Type of data | Tables, figures, text files |
| How data was acquired | Two-detector setup with plastic scintillators in co-linear (180°) arrangement using the DRS4 evaluation board for digitization (acquisition software: DRRS4PALS v1.04) |
| Data format | Raw spectra |
| Experimental factors | Lifetime spectrum acquisition:  
  sample: tin (4N-Sn) annealed at 250 °C (5 h)  
  source: $^{22}$Na (25μCi, 9.25 × 10$^8$Bq) sealed in Kapton foil  
Prompt spectrum acquisition:  
  source: $^{60}$Co (1μCi, 3.7 × 10$^8$Bq) |
| Experimental features | The radioactive source $^{22}$Na was sandwiched between two identical tin samples (4N-Sn) (source-sample sandwich) |
| Data source location | University Wuerzburg, Department of Chemistry and Pharmacy, LCTM Roentgenring 11, D-97070 Wuerzburg |
| Data accessibility | Data is with this article |
| Related research article | N/A |

### Value of the data

- This completely transparent documentation of the experiment with respect to the setup, acquisition process and data reduction enables reproducibility by other research groups.
- Since reference values for specific bulk lifetimes of pure metals have a wide scatter in literature, the here provided experimentally obtained spectra can be taken to verify data acquired on pure tin samples.
- The here provided simulated spectra allow to verify the validity and functionality as well as the sensitivity and correctness of the algorithms (or software) used to decompose the relevant information, i.e. characteristic/specific lifetime and intensity.
- The simulated spectra allow to determine the maximum provided information content given by experimentally obtained spectra.
- The knowledge of the reference specific bulk lifetimes is crucial to obtain the correct source correction and, thus, to reduce artifacts in the following data treatment.

### 1. Data

The hereby provided data are divided into three collections, where collection 1 (ED1) and collection 2 (SD1) correspond to the experimentally obtained and simulated positron annihilation lifetime spectra of pure tin (4N-Sn), respectively. We use equivalent settings, which are shared in two files (settingsExp.drs4LTSettings and settingsSim.drs4LTSettings). Each collection ED1 and SD1 contains a set of six lifetime spectra with various statistics (500k, 1000k, 1500k, 2000k, 2500k and 2800k counts) acquired. The input of the simulated lifetime spectra (SD1) was derived from the retrieved specific lifetimes and its intensities of the experimentally obtained lifetime spectra (ED1) as an outcome of the least-square fitting procedure [2].

Furthermore, ED1 contains the data of the quasi instrument response function (IRF), i.e. the prompt spectrum, recorded using $^{60}$Co with an activity of 1μCi (3.7 × 10$^8$Bq) (specExp_co60.dat). Additionally, the pulse height spectra (PHS) are provided. A third collection (Conf1) comprehends two setting files related to the type of data acquisition, i.e. the simulation or acquisition mode, using
DDRS4PALS software [3]. The parameters most relevant for the timing determination using the constant fraction principle are equal for both, the acquisition of the experimentally obtained and simulated spectra. Nevertheless, the setting files are separated into experiment (settingsExp.drs4LTSettings) and simulation (settingsSim.drs4LTSettings). The simulation input file, used for the spectra simulation, is included in Conf1. A detailed overview of the data structure is given in Table 1.

| collection | name of file | brief description |
|------------|-------------|-------------------|
| ED1        | specExp_500k.dat | experimentally obtained lifetime spectrum (500k counts) |
|            | specExp_1000k.dat | |
|            | specExp_1500k.dat | |
|            | specExp_2000k.dat | |
|            | specExp_2500k.dat | |
|            | specExp_2800k.dat | |
|            | phs_A.dat | pulse height spectrum (PHS - detector A) |
|            | phs_B.dat | pulse height spectrum (PHS - detector B) |
|            | specExp_co60.dat | experimentally obtained prompt spectrum using $^{60}$Co |
|            | phs_A_co60.dat | pulse height spectrum (PHS - detector A) using $^{60}$Co |
|            | phs_B_co60.dat | pulse height spectrum (PHS - detector B) using $^{60}$Co |
| SD1        | specSim_500k.dat | simulated lifetime spectrum (500k counts) |
|            | specSim_1000k.dat | |
|            | specSim_1500k.dat | |
|            | specSim_2000k.dat | |
|            | specSim_2500k.dat | |
|            | specSim_2800k.dat | |
| Conf1      | settingsExp.drs4LTSettings | experiment: settings file (DDRS4PALS software) |
|            | settingsSim.drs4LTSettings | simulation: settings file (DDRS4PALS software) |
|            | simulationSn.drs4SimulationInputFile | simulation input file (DDRS4PALS software) |

2. Experimental design, materials and methods

2.1. Experimental setup

The positron lifetime measurements were carried out using the semi-digital/analog setup as shown in Fig. 1. The setup can be divided into the photo detection system (Section 1.1), an analog (Section 1.2) and a digital (Section 1.3) hardware section. Non-coincide events are pre-filtered by the analog section, whereas coincident events prompt the DRS4 evaluation board [1] (digital section) for digitization of the photomultiplier’s dynode output pulses by an external trigger signal originated from the coincidence unit. Furthermore, the digitized pulses are processed using the software tool DDRS4PALS [3].

2.1.1. Photo detection system

The photo detection system consists of two co-linearly (180°) arranged Hamamatsu (H1949-50/WA-5309) photomultiplier tubes (Fig. 1: PMT A and B) with conically shaped¹ ultra-fast BC422Q (0.5 wt.% benzophenone) scintillators (Fig. 1, right). The PMTs A and B are separately power supplied by two high voltage units (Table 8), set to -2.09 kV and -2.11 kV, respectively. The scintillators are directly attached to the PMT faceplates using Wacker silicone oil (AK 10,000) to provide an optimal optical transition.

¹ The conically shaped scintillators allow a close arrangement of multiple detectors around the source-sample sandwich (Section 2).
As displayed in Fig. 1, the anode outputs of the PMTs are connected to the constant fraction discriminators (CFD) of the analog section (1.2), whereas the dynode outputs are connected to the analog inputs of the DRS4 evaluation board (1.3).

2.1.2. Acquisition hardware: analog section

As shown in Fig. 1, the analog section consists of two constant fraction discriminators (CFD) for each analog output of the photomultiplier tubes (PMT) A and B, and a coincidence unit, whose output serves as external trigger signal for the DRS4 evaluation board (digital section). The external trigger prompts the digitization of the dynode output pulses. Since both standard pulses of CFD A and B fall into the coincidence window of 2 $\mu$s, a rectangular shaped pulse is emitted by the coincidence unit and serves as external trigger signal for the DRS4 evaluation board to start the readout operation and digitization of the respective dynode pulses. Finally, the output signal of the coincidence unit is attenuated by -30 dB to fit the external trigger input range of the DRS4 evaluation board.

2.1.3. Acquisition hardware: digital section

Once the DRS4 evaluation board received the external trigger, the domino wave starts charging the switched capacitor arrays successively with the sampled voltages of the dynode output pulses (see principle of DRS4 chip [1]) using a sampling rate of 5.12 GHz with a sweep of 200 ns (Table 3). This leads to an average sampling increment of 195 ps for 1024 sampling points (capacitors). Subsequently, the stored pulses are digitized by an 80MHz ADC (14 bit) and read out via USB 2.0. Moreover, the pulses are attenuated by -20dB before connecting to the DRS4 evaluation board to fit the analog input

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**Table 2**

Listing of the used analog hardware components regarding Fig. 1.

| analog: hardware component                  | type                              | supplier/manufacturer |
|---------------------------------------------|-----------------------------------|----------------------|
| constant fraction discriminator (CFD)       | CFD Diff Disc (583)               | Ortec                |
| coincidence unit                           | Universal Coincidence (418A)      | Ortec                |
| high voltage (HV)                          | High Voltage Supply (556)         | Ortec                |
| photomultiplier tube (PMT)                 | H1949-50/WA-5309                  | Hamamatsu            |
| scintillator crystal                       | BC422Q (0.5 wt.% benzophenone)    | Bicron/Saint-Gobain  |

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As displayed in Fig. 1, the anode outputs of the PMTs are connected to the constant fraction discriminators (CFD) of the analog section (1.2), whereas the dynode outputs are connected to the analog inputs of the DRS4 evaluation board (1.3).

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**Fig. 1.** Left: Schematic illustration of the semi-digital/analog setup used for the acquisition of the lifetime and prompt spectra (Fig. 6). The analog section consists of two constant fraction discriminators (CFD) for each analog output of the photomultiplier tubes (PMT) A and B, and a coincidence unit, whose output serves as external trigger signal for the DRS4 evaluation board (digital section). The external trigger prompts the digitization of the dynode output pulses. Right: Geometry and dimensions of the conically shaped BC422Q (0.5% benzophenone) scintillator crystals, which are attached on the PMT’s faceplate.
range of ±500 mV. Before data acquisition, the DRS4 evaluation board was voltage and timing calibrated to reduce noise using the DRS0sc software [4]. The evaluation board enables a convenient way of software-based pulse processing, as it was shown elsewhere by Petriska et al. [5] and Bin et al. [6].

2.2. Sample preparation

Two tin (4N-Sn, Advent Research Materials Ltd.) plates of equivalent dimensions 10×10×1 mm were annealed at 250 °C for 5 h without vacuum or protective gas flow. Hence, the defect density (dislocations and vacancies) is reduced below the detection limit for positrons in metals [7] and the specific bulk lifetime outweighs. $^{22}\text{Na}$ with an activity of 25μCi (9.25×10⁵Bq) serves as positron source and is covered by two Kapton foils with a combined thickness of approximately 15 μm (Fig. 2). Moreover, the Kapton foils are fixed by a thin ring of glue. For measurement, the positron source is centered between the tin samples, which is commonly described as source-sample sandwich. To avoid a displacement between the source and samples during the measurement, the sandwich was wrapped into household aluminium foil.

2.3. Acquisition of lifetime spectra

The hereby provided positron lifetime spectra (Table 1), were obtained using the software tool DDRS4PALS v1.04 [3]. The channel width (binning) was chosen to be 5 ps (10,000 channels/bins upon 50 ns).

DDRS4PALS can be executed in two modi, the acquisition and the simulation mode. The acquisition mode processes the dynode output pulses, recorded and digitized by the DRS4 evaluation board, whereas the simulation mode is based on the C++ library DLTPulseGenerator [8–10] which provides the simulation of lifetime spectra according to the measurement setup.

However, for both types of lifetime spectra, i.e. the experimental and the simulated, the equivalent parameter values, as stored in the setting files settingsExp.drs4LTSettings and settingsSim.

| digital: DRS4 evaluation board settings | value |
|----------------------------------------|-------|
| sampling rate                          | 5.12 GHz |
| number of cells/sweep                  | 1024 (200 ns) |
| analog input range                     | ±500 mV |
| trigger type                           | external |
| evaluation board type                  | 9     |
| firmware version                       | 21305 |

Table 3
Listing of the used DRS4 evaluation board settings.

Fig. 2. Left: Illustration of the source-sample sandwich. Right: Geometry of the positron source covered by Kapton foils.
Table 4  
Listing of the parameters, most relevant for the timing determination.

| pulse timing determination | value |
|---------------------------|-------|
| signal output             | dynode|
| pulse rise time           | 2.5 ns|
| d-CFD level A             | 25%   |
| d-CFD level B             | 25%   |
| algorithm type for d-CFD  | cubic spline interpolation (ALGLIB [11]) |

Table 5  
Listing of the pulse height spectra (PHS) windows of detector A and B used for the energy selection of start and stop events (see coloured frames in Fig. 4).

| pulse height spectrum (PHS): A | value |
|-------------------------------|-------|
| start (LL)                    | 230 mV|
| start (UL)                    | 454 mV|
| stop (LL)                     | 78 mV |
| stop (UL)                     | 107 mV|

| pulse height spectrum (PHS): B | value |
|-------------------------------|-------|
| start (LL)                    | 231 mV|
| start (UL)                    | 466 mV|
| stop (LL)                     | 84 mV |
| stop (UL)                     | 116 mV|

drs4LTSettings, were applied. The parameters, most relevant for the timing determination (Section 3.1) and the pulse height discrimination (Section 3.2), are listed in Tables 4 and 5.

2.3.1. Pulse timing

The software-based constant fraction principle (d-CFD) was accomplished to determine the correct timing of the digitized dynode output pulses using a d-CFD level of 25% for both branches A and B. A cubic spline interpolation (ALGLIB [11]) of the sample points was applied before the d-CFD determination to provide a smooth pulse shape. The d-CFD value was calculated from the spline interpolated maximum (amplitude) without applying prior corrections on the baseline. The rising edge includes approximately ten sampling points, as displayed in the orange shaded region in Fig. 3.

For the simulated lifetime spectra, the rise-time of the modelled detector output pulses was set to 2.5 ns (see file simulationSn.drs4SimulationInputFile), as this is the rise-time of the dynode output pulses (Fig. 3).

2.3.2. Pulse height discrimination

The PHS windows, as specified in Table 5, of detector A and B (Fig. 1) are used for the energy selection of start (Fig. 4, green frame) and stop (Fig. 4, red frame) events. They are identical for the acquisition of the lifetime and prompt spectra.

To reduce the data transfer rate through the USB 2.0 interface and, hence, preventing the digitization of negligible events, the lower level (LL) of the CFD window was shifted to pulse heights (amplitude) close to the LL of the stop window (Fig. 4, red frame) in the PHS, as it is indicated by the red line in Fig. 4. Further performance improvements can be achieved by using only one combination of start and stop branch (e.g. A as start and B as stop). Therefore, the digitization can be significantly

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2 The data transfer rate of USB 2.0 is limited to 25 Mbyte/s. The data size of each digitized pulse pair (detector A and B) is 16 kByte = 1024 (readout cells) × 2 (time and voltage of A) × 2 (time and voltage of B) × 4 (size of data type float in bytes). Therefore, the efficiency is limited to approximately 500 pulse pairs/s (see also [5]).
Fig. 3. Digitized PMT (Hamamatsu of type H1949-50/WA-5309) dynode output pulse (blue dots): The red line indicates the cubic spline interpolated output pulse, whereas the orange shaded frame represents the region relevant for the timing determination using the software-based constant fraction principle (d-CFD). The rise-time of the dynode output pulses is approximately 2.5 ns. No prior corrections on the baseline were applied.

Fig. 4. Pulse height spectra (PHS) of scintillators BC422Q (0.5% benzophenone) for $^{22}$Na (top) and $^{60}$Co (bottom). The coloured frames indicate the energy windows of the start (green) and stop (red) events. The red line represents the lower level (LL) of the constant fraction discriminator in the analog section (CFD, Fig. 1) and specifies the minimum accepted amplitude (red line).
reduced by adapting the lower (LL) and upper level (UL) of the CFD windows to the relevant pulse heights (amplitude) in the PHS only.

However, the PHS, as shown in Fig. 5, are related to the files phs_A.dat/phs_B.dat and phs_A_co60.dat/phs_B_co60.dat.

2.3.3. Pulse filtering: area filter

Pile-up events were rejected by applying a pulse area filter on both branches A and B, as shown in Fig. 5, which essentially leads to an improved spectra quality. For the measurement of the quasi instrument response function (IRF) using $^{60}$Co (Fig. 6), the same windows were applied (see file settingsExp.drs4LTSettings).

2.4. Lifetime spectra analysis

The experimentally obtained and simulated lifetime spectra were analysed (Tables 8, 9 and 11, 12) using the software tool $D$QuickLT$Fit$ v4.0 [12]. The employed fit model is the commonly used analytical solution of the convolution of a sum of N exponential distributions with a sum of gaussian distribution functions, as first published by Kirkegaard et al. [2]. Moreover, $D$QuickLT$Fit$ has implemented the MPFIT library [13] for solving the non-linear least-square problem using the Levenberg-Marquardt algorithm [14,15]. The analysis was performed on

(1) the initial lifetime spectra, acquired with a channel width of 5 ps (bin factor: 1, Tables 8 and 11), and

(2) the re-binned lifetime spectra, by applying a bin-factor of ten, which results in a channel width of 50 ps (bin factor: 10, Tables 9 and 12).
Fig. 6. Experimentally obtained positron lifetime spectra (red dots) for different statistics acquired measuring pure tin (4N-Sn). The number of used channels is 10,000 with a channel width of 5 ps. Moreover, the blue line indicates the best fit. The quasi instrument response function (IRF – prompt spectrum) was measured using $^{60}$Co (1μCi). Subsequently, a FWHM of (204.8 ± 0.5) ps was determined using a single Gaussian fit as guide for the eye.
2.4.1. Experimentally obtained lifetime spectra

For the spectra analysis in high-purity, well annealed samples, three specific lifetimes, originating from

- the bulk material (in this case tin, 4N-Sn),
- the $^{22}$Na salt and the Kapton foil (combined),
- and the formed positronium

are expected to be extracted from the experimentally obtained lifetime spectra. The fitting parameters and start values of the expected specific lifetimes and its corresponding intensities were used for both types of lifetime spectra: the experimentally obtained and the simulated. The shortest component ($\tau_1/I_1$) relates to the bulk (tin), whereas the other contributions, i.e. $\tau_2/I_2$ and $\tau_3/I_3$, relate to the Kapton foil and $^{22}$Na (salt) in combination, and positronium, which is probably forming at interfaces between source and source covering foil (see Fig. 2).

| Value       |       |
|-------------|-------|
| $\tau_1$ [ps] | 198   |
| $I_1$       | 0.900 |
| $\tau_2$ [ps] | 380   |
| $I_2$       | 0.100 |
| $\tau_3$ [ps] | 2200  |
| $I_3$       | 0.005 |
| $G_1$: FWHM [ps] | 198   |
| $G_1$: $I_1$ | 0.5   |
| $G_2$: FWHM [ps] | 198   |
| $G_2$: $I_2$ | 0.5   |

### Table 6

Parameters used for the least-square fitting procedure of the experimentally obtained and simulated lifetime spectra. The fit was applied on the lifetime spectra for the binning factors one and ten which results in a channel width of 5 ps and 50 ps, respectively.

| bin factor: 1 (channel width: 5 ps) | least-square fitting parameters |
|-------------------------------------|---------------------------------|
| ROI [start:stop]                   | [329:9480]                     |
| channel region: background calculation | [7481:9480] = 2000          |
| fixed background?                  | no                             |
| fit weighting                      | $w_i = y_i^{-1/2}$             |

| bin factor: 10 (channel width: 50 ps) | least-square fitting parameters |
|--------------------------------------|---------------------------------|
| ROI [start:stop]                    | [33:948]                        |
| channel region: background calculation | [749:948] = 200                |
| fixed background?                   | no                             |
| fit weighting                       | $w_i = y_i^{-1/2}$              |

### Table 7

Start values of the least-square fitting procedure used for determination of the specific lifetimes and its intensities as well as the instrument response function (IRF) using a superposition of two Gaussian functions ($G_1/G_2$). The start values for the specific lifetimes and corresponding intensities were used for both types of lifetime spectra: the experimentally obtained and the simulated. The shortest component ($\tau_1/I_1$) relates to the bulk (tin), whereas the other contributions, i.e. $\tau_2/I_2$ and $\tau_3/I_3$, relate to the Kapton foil and $^{22}$Na (salt) in combination, and positronium, which is probably forming at interfaces between source and source covering foil (see Fig. 2).
2.4.2. Simulated lifetime spectra

The retrieved specific lifetimes $\tau_i$ and corresponding intensities $I_i$ and the FWHM, contributions $c$ and relative shifts $\Delta t$ to $t_0 = 5468$ ps of the modelled Gaussian IRFs ($G_1/G_2$) at different counts acquired using a least-square fit. The bracketed values indicate the standard errors of the fitted values.

| acquired counts | $\tau_1$ [ps] | $I_1$ | $\tau_2$ [ps] | $I_2$ | $\tau_3$ [ps] | $I_3$ |
|-----------------|---------------|-------|---------------|-------|---------------|-------|
| 500k            | 196.9         | 0.862 | 423           | 0.1337| 3904          | 0.00470|
|                 | (3.8)         | (0.029)| (22)          | (0.0029)| (559)       | (0.00040)|
| 1000k           | 197.0         | 0.864 | 429           | 0.1312| 4535          | 0.00520|
|                 | (2.7)         | (0.019)| (15)          | (0.0019)| (414)       | (0.00030)|
| 1500k           | 194.3         | 0.842 | 405           | 0.1530| 3658          | 0.00530|
|                 | (2.7)         | (0.020)| (13)          | (0.0024)| (270)       | (0.00030)|
| 2000k           | 194.6         | 0.837 | 399           | 0.1570| 3269          | 0.00570|
|                 | (2.4)         | (0.019)| (11)          | (0.0023)| (202)       | (0.00020)|
| 2500k           | 192.6         | 0.8236| 387           | 0.1706| 3053          | 0.00580|
|                 | (2.5)         | (0.0191)| (10)         | (0.0026)| (170)       | (0.00020)|
| 2800k           | 191.9         | 0.8192| 384.9         | 0.1750| 3062          | 0.00580|
|                 | (2.4)         | (0.0182)| (9.3)        | (0.0026)| (158)       | (0.00020)|

|               | $G_1$: FWHM [ps] | $G_1$: $c$ | $G_1$: $\Delta t$ [ps] | $G_2$: FWHM [ps] | $G_2$: $c$ | $G_2$: $\Delta t$ [ps] |
|---------------|-----------------|------------|------------------------|-----------------|------------|------------------------|
| 500k          | 192.6           | 0.899      | 2.64                   | 301             | 0.101      | –21                    |
|               | (2.8)           | (0.040)    | (0.89)                 | (13)            | (0.040)    | (25)                   |
| 1000k         | 195.4           | 0.922      | 3.14                   | 311             | 0.0783     | –23                    |
|               | (1.8)           | (0.027)    | (0.60)                 | (12)            | (0.027)    | (24)                   |
| 1500k         | 197.6           | 0.937      | 1.15                   | 328             | 0.063      | –23                    |
|               | (1.3)           | (0.019)    | (0.44)                 | (13)            | (0.019)    | (25)                   |
| 2000k         | 198.1           | 0.945      | 0.81                   | 317             | 0.055      | –40                    |
|               | (1.3)           | (0.021)    | (0.42)                 | (15)            | (0.021)    | (33)                   |
| 2500k         | 198.2           | 0.942      | 0.80                   | 326             | 0.058      | –31                    |
|               | (1.1)           | (0.017)    | (0.35)                 | (12)            | (0.017)    | (24)                   |
| 2800k         | 198.5           | 0.944      | 0.83                   | 328             | 0.057      | –30                    |
|               | (1.0)           | (0.015)    | (0.33)                 | (11)            | (0.015)    | (23)                   |

2.4.2. Simulated lifetime spectra

The retrieved specific lifetimes and their corresponding intensities of the experimentally obtained lifetime spectrum with bin factor: 1 (channel width: 5 ps): the specific lifetimes $\tau_i$ and the FWHM, contributions $c$ and relative shifts $\Delta t$ to $t_0 = 5468$ ps of the modelled Gaussian IRFs ($G_1/G_2$) at different counts acquired using a least-square fit. The bracketed values indicate the standard errors of the fitted values.
Table 9
Retrieved relevant parameters of the experimentally obtained lifetime spectra with bin factor: 10 (channel width: 50 ps): the specific lifetimes $\tau_i$ and corresponding intensities $I_i$ and the FWHM, contributions $c$ and relative shifts $\Delta t_0 = 5468$ ps of the modelled Gaussian IRFs ($G_1/G_2$) at different counts acquired using a least-square fit. The bracketed values indicate the standard errors of the fitted values.

| acquired counts | $\tau_1$ [ps] | $I_1$   | $\tau_2$ [ps] | $I_2$   | $\tau_3$ [ps] | $I_3$   |
|-----------------|--------------|--------|--------------|--------|--------------|--------|
| 500k            | 194.0        | 0.841  | 406          | 0.1522 | 4083         | 0.00550|
|                 | (4.6)        | (0.025)|(21)         | (0.0039)| (474)        | (0.00040)|
| 1000k           | 196.3        | 0.858  | 424          | 0.1362 | 4343         | 0.00530|
|                 | (2.9)        | (0.015)|(15)         | (0.0021)| (391)        | (0.00030)|
| 1500k           | 191.9        | 0.824  | 389          | 0.1706 | 3416         | 0.00570|
|                 | (3.1)        | (0.023)|(13)         | (0.0032)| (237)        | (0.00030)|
| 2000k           | 193.7        | 0.831  | 393          | 0.1632 | 3209         | 0.00580|
|                 | (2.5)        | (0.020)|(11)         | (0.0026)| (194)        | (0.00030)|
| 2500k           | 191.9        | 0.818  | 384          | 0.175  | 3051         | 0.00590|
|                 | (2.5)        | (0.016)|(10)         | (0.016)| (167)        | (0.00020)|
| 2800k           | 191.5        | 0.817  | 383.4        | 0.1777 | 3056         | 0.00590|
|                 | (2.4)        | (0.018)|(9.5)        | (0.0027)| (159)        | (0.00030)|

|               | $G_1$: FWHM [ps] | $G_1$: $c$ | $G_1$: $\Delta t$ [ps] | $G_2$: FWHM [ps] | $G_2$: $c$ | $G_2$: $\Delta t$ [ps] |
|---------------|------------------|-----------|------------------------|------------------|-----------|------------------------|
| 500k          | 195.5            | 0.929     | –2.59                  | 332              | 0.071     | –24                    |
|               | (2.2)             | (0.031)   | (0.71)                 | (19)             | (0.031)   | (36)                   |
| 1000k         | 196.7            | 0.936     | –1.81                  | 321              | 0.064     | –34                    |
|               | (1.8)             | (0.026)   | (0.58)                 | (16)             | (0.026)   | (32)                   |
| 1500k         | 197.7            | 0.933     | –3.75                  | 332              | 0.067     | –21                    |
|               | (1.3)             | (0.019)   | (0.43)                 | (12)             | (0.019)   | (22)                   |
| 2000k         | 198.1            | 0.944     | –4.19                  | 320              | 0.057     | –41                    |
|               | (1.3)             | (0.021)   | (0.42)                 | (14)             | (0.021)   | (31)                   |
| 2500k         | 198.4            | 0.941     | –4.16                  | 327              | 0.059     | –34                    |
|               | (1.1)             | (0.017)   | (0.36)                 | (12)             | (0.017)   | (24)                   |
| 2800k         | 198.6            | 0.943     | –4.17                  | 330              | 0.057     | –34                    |
|               | (1.0)             | (0.015)   | (0.33)                 | (11)             | (0.015)   | (23)                   |

Table 10
Specific lifetimes and its intensities, which served as simulation input (see file "simulationSn.drs4SimulationInput"). As the instrumental response (IRF), a single Gaussian with a FWHM corresponding to the effective FWHM (condition: $\Delta t = 0$ ps) of the experimentally obtained spectrum with the highest statistics (2.8 million counts, Table 8) acquired, was taken.

| simulation input | value   |
|------------------|---------|
| $\tau_1$ [ps]    | 192     |
| $I_1$            | 0.82    |
| $\tau_2$ [ps]    | 385     |
| $I_2$            | 0.175   |
| $\tau_3$ [ps]    | 3050    |
| $I_3$            | 0.005   |
| FWHM [ps]        | 205     |
Table 11
Simulated lifetime spectra with bin factor: 1 (channel width: 5 ps): Retrieved specific lifetimes and its corresponding intensities for different counts acquired using a least-square fit. The bracketed values indicate the standard errors of the fitted values.

| acquired counts | $\tau_1$ [ps] | $I_1$ | $\tau_2$ [ps] | $I_2$ | $\tau_3$ [ps] | $I_3$ | FWHM [ps] |
|-----------------|---------------|-------|---------------|-------|---------------|-------|-----------|
| 500k            | 194.6 (2.8)   | 0.836 | 395 (18)      | 0.1607 | 2954 (528)    | 0.0036 | 204.27    |
| 1000k           | 192.4 (2.0)   | 0.824 | 388 (12)      | 0.1713 | 2858 (259)    | 0.0046 | 204.91    |
| 1500k           | 192.7 (1.7)   | 0.824 | 387.5 (9.3)   | 0.1715 | 3083 (207)    | 0.0049 | 205.07    |
| 2000k           | 192.3 (1.4)   | 0.820 | 385.1 (8.0)   | 0.1751 | 3096 (175)    | 0.0049 | 205.21    |
| 2500k           | 191.5 (1.3)   | 0.815 | 381.1 (7.1)   | 0.1804 | 3022 (151)    | 0.0050 | 205.42    |
| 2800k           | 190.3 (1.3)   | 0.804 | 374.0 (7.6)   | 0.1907 | 2883 (133)    | 0.0052 | 205.58    |

Table 12
Simulated lifetime spectra with bin factor: 10 (channel width: 50 ps): Retrieved specific lifetimes and its corresponding intensities for different counts acquired using a least-square fit. The bracketed values indicate the standard errors of the fitted values.

| acquired counts | $\tau_1$ [ps] | $I_1$ | $\tau_2$ [ps] | $I_2$ | $\tau_3$ [ps] | $I_3$ | FWHM [ps] |
|-----------------|---------------|-------|---------------|-------|---------------|-------|-----------|
| 500k            | 195.2 (2.6)   | 0.841 | 402 (16)      | 0.1547 | 3500 (440)    | 0.00430 | 204.36    |
| 1000k           | 192.6 (1.9)   | 0.826 | 390 (11)      | 0.1695 | 3090 (254)    | 0.00480 | 204.90    |
| 1500k           | 192.8 (1.6)   | 0.826 | 389.5 (9.2)   | 0.1696 | 3172 (208)    | 0.00490 | 205.11    |
| 2000k           | 192.4 (1.4)   | 0.821 | 385.4 (8.0)   | 0.1745 | 3083 (173)    | 0.00500 | 205.20    |
| 2500k           | 191.8 (1.3)   | 0.817 | 382.9 (7.1)   | 0.1782 | 3077 (154)    | 0.00500 | 205.37    |
| 2800k           | 190.5 (1.3)   | 0.806 | 375.0 (6.6)   | 0.1893 | 2961 (136)    | 0.00520 | 205.54    |

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Transparency document. Supporting information

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.121.

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