Identification and simulation of surface alpha events on passivated surfaces of germanium detectors and the influence of metalisation

I. Abt, C. Gooch, F. Hagemann, L. Hauertmann, X. Liu, O. Schulz, M. Schuster, A. J. Zsigmond
Max Planck Institut für Physik, Föhringer Ring 6, 80805 Munich, Germany

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Abstract

Events from alpha interactions on the surfaces of germanium detectors are a major contribution to the background in germanium-based searches for neutrinoless double-beta decay. Surface events are subject to charge trapping, affecting their pulse shape and reconstructed energy. A study of alpha events on the passivated end-plate of a segmented true-coaxial n-type high-purity germanium detector is presented. Charge trapping is analysed in detail and an existing pulse-shape analysis technique to identify alpha events is verified with mirror pulses observed in the non-collecting channels of the segmented test detector. The observed radial dependence of charge trapping confirms previous results. A dependence of the probability of charge trapping on the crystal axes is observed for the first time. A first model to describe charge trapping effects within the framework of the simulation software SolidStateDetectors.jl is introduced. The influence of metalisation on events from low-energy gamma interactions close to the passivated surface is also presented.

1 Introduction

High-purity germanium (HPGe) detectors are well suited to search for physics beyond the Standard Model such as neutrinoless double-beta ($0\nu\beta\beta$) decay [1–5] and dark matter [6–8]. In such rare-event searches, it is essential to suppress background events as much as possible.

The LEGEND experiment [1,5] will search for $0\nu\beta\beta$ decay in $^{76}\text{Ge}$ using HPGe detectors based on the experience of the preceding experiments GERDA [4,9] and MAJORANA DEMONSTRATOR [3,10]. In these experiments, a substantial part of the background events with observed energies close to the $Q$-value of the $0\nu\beta\beta$ decay ($Q_{\beta\beta} = 2039$ keV) originates from events near the surface of the detectors [11]. Pulse-shape discrimination techniques have been developed to reject such surface events [12], including a dedicated method to identify events originating from the large passivated surfaces of the point-contact detectors of the MAJORANA DEMONSTRATOR [13]. A substantial further reduction of background is essential for LEGEND to reach its goal of increasing the half-life sensitivity to $0\nu\beta\beta$ decay of $^{76}\text{Ge}$ to $10^{28}$ years and beyond [5]. A deep understanding of the HPGe detectors and their signal pulses is essential to achieve this.

A study of alpha events on the passivated surface of the segmented true-coaxial n-type HPGe detector, “Super-Siegfried” [14], was performed in the GALATEA test facility [15] at the Max Planck Institute for Physics in Munich. Such events are an important background to $0\nu\beta\beta$ decay searches when charge trapping reduces the observed energy to values within the region of interest around $Q_{\beta\beta}$ [11].

For the first time, the dependence of charge trapping on the orientation of the crystal axes is presented. First attempts to simulate surface effects with the open-source software package SolidStateDetectors.jl [16] are also shown.

In general, all contacts of germanium detectors are completely coated with a thin metal layer, i.e. are fully metalised. However, the segments of the detector Super-Siegfried were originally not fully metalised but were only partially metalised on a dedicated contact area. The results of studies [14] where data were taken with partially metalised contacts were compared to results from data taken after the segments became fully metalised. The influence of the extent of the metalisation is demonstrated.

2 Experimental setup and data taking

GALATEA is based on a vacuum chamber in which the top and side surfaces of a detector can be scanned using a system of three motorised stages, see Fig. 1.
The HPGe detector is mounted on a holder, which is cooled via a copper cooling finger submerged in an integrated liquid-nitrogen tank. The fill level of the tank is monitored and the internal tank is automatically refilled through a connected dewar.

The special feature of GALATEA is that the path between the detector and the source is free of material, facilitating the use of alpha sources. Two sources can be mounted in two tungsten collimators focusing the radiation onto the mantle and top plate of the detector, respectively. The collimators are moved by linear stages and slide along slits on the side and top of a silver-coated copper hat serving as an infrared shield. A rotational stage moves these components around the detector, such that almost any point on the detector top surface or mantle can be irradiated. Significant improvements of the setup since previous studies [14], such as stable long-time operation, automated data taking and the use of open alpha sources, allowed for more detailed studies of charge trapping.

Two open alpha $^{241}$Am sources, each with an activity of 74 kBq, were installed in the two collimators allowing for simultaneous scans of the side and the top of the detector. The isotope $^{241}$Am decays into $^{237}$Np with dominant alpha energies of $Q_{\alpha_1} = 5485.6$ keV, $Q_{\alpha_2} = 5442.8$ keV and $Q_{\alpha_3} = 5388.2$ keV [17]. In addition, $^{237}$Np emits 59.5 keV gammas. The alphas lose their energy within 20 µm of germanium with the Bragg peak at 17 µm [18] and create events directly underneath the surface of the detector. Figure 2 shows the observed spectrum in response to irradiation from the side. The reduction of the observed energies with respect to the emitted energies corresponds to the contact thickness on the side of the detector. The width of the observed lines arises from self-absorption in the source.

Super-Siegfried is a cylindrical true-coaxial n-type segmented HPGe detector produced by Canberra France, now Mirion Technologies [19]. The detector has a height of 70 mm, an outer radius of 37.5 mm and a borehole with a radius of 5 mm. At the top and the bottom, the borehole widens to a radius of 10 mm within about 3 mm. The impurity density as stated by the manufacturer of the crystal is $0.44 \times 10^{10}$ cm$^{-3}$ at the top and $1.30 \times 10^{10}$ cm$^{-3}$ at the bottom. The recommended operational voltage is 3000 V.

The lithium-drifted inner surface of the borehole (not including the area of the widening) is the only n$^+$ contact, the so-called core contact. The outer mantle is segmented into 19 p$^+$ contacts produced via boron implantation, see Fig. 3a. The 18 lower segments are ordered in a $6 \times 3$ geometry in $\phi$ and $z$. These segments are read-out at their centres via

![Fig. 1](image_url)  
**Fig. 1**  
(a) An illustration adapted from [15] and (b) a photo of the vacuum chamber of GALATEA with the main components marked in (a). (c) Schematic of the central part of GALATEA with the infrared (IR) shield and the top collimator and an illustration of the beam-spot.
Fig. 3  a Side view: the segment structure of the mantle of Super-Siegfried with dimensions and reference coordinate system. b Top view: the positions of the measurements on the top surface are marked. Also shown are the crystal axes in a and b. The framed numbers denote the segments numbers, in b for the segments underneath segment 19.

one Kapton printed-circuit-board [20]. An additional segment located above these 18 segments, segment 19, has a height of 5 mm and is not segmented in $\phi$. It is read out via a cable at $\phi_{10} \approx 135^\circ$, see Fig. 3. Prior to the full metalisation, the read-out cable for segment 19 was connected at about the same location. The detector, as ready to be mounted on the cooling finger in GALATEA, is depicted in Fig. 4. The fairly thin segment 19 was designed to study events on the passivated surface of the top end-plate. Charges drifting towards the segment 19 contact also create strong so-called mirror pulses in the segments underneath, which facilitate a detailed pulse-shape analysis.

The positions of the two sources were calibrated by moving the collimators and identifying the segment boundaries and the crystal axes as well as the relative position of the holding structure [18]. Figure 3b shows the position of the $\langle 100 \rangle$ and $\langle 110 \rangle$ crystal axes, referred to as fast and slow axes, respectively, as the charge carriers drift faster and slower along these axes in germanium. All events recorded for a given position of the sources are from here on called a measurement. All positions refer to the positions of the centre of the beam-spot on the detector surface. The individual measurement positions on the top and side of the detector are also shown in Fig. 3. They comprise two radial scans, RSF along a fast axis and RSS along a slow axis, and two rotational (azimuthal) scans, AST from the top at a fixed radius of 23.8 mm and from the side at $z = 40$ mm and ASS only from the side on segment 19. The index $j$ is used throughout this paper to refer to the $j$-th measurement of the respective scan. Each measurement of these four scans lasted one hour. In addition, a five hour long background measurement (BG) was performed where the sources did not irradiate the detector.

The alpha beam from the top as provided by the setup was simulated with Geant4 [21] to investigate the incident spectrum and beam-spot on the top surface. A simulation
of monoenergetic 5.485 MeV alphas from the source in the top collimator showed that the resulting spectrum has a tail towards low energies, see Fig. 5. This tail is populated by alphas which loose energy through interactions with the wall of the collimator or the edge of the slit in the infrared shield. The shape and population of the beam-spot is shown in Fig. 6. The sharp cut-off, perpendicular to the radial direction, is caused by the additional collimation provided by the infrared shield.

For a single event, 20 pulses (from the core and all 19 segments), each with 5000 samples, were recorded with a sampling rate of 250 MHz by two 16-channel Struck SIS3316 [22] analog-to-digital converter units. The index $i \in [0, 19]$ is used throughout this paper to specify the channel. All devices of GALATEA were controlled and monitored via one software package, which allowed for automated scans of the detector. The trigger was provided by the core channel connected to the first unit which forwarded its trigger signal to the second unit via a short cable. The constant time delay of the second unit was taken into account in the offline pulse processing [18].

A typical raw (prior to any processing) pulse, from the core channel is shown in Fig. 7a.

This included a correction for the decay of charge in the preamplifier of each channel $i$ [23]. After baseline subtraction, an exponential function, $e^{-t/\tau_i}$, was fitted to the part of each pulse following the rise, the so-called tail. For all measurements, the characteristic decay constants of each preamplifier, $\tau_i$, were determined by fitting a Cauchy function to the $\tau_i$-distributions for bulk events [23]. The pulse shown in Fig. 7a is shown in Fig. 7b after cross-talk correction and calibration. All pulses were corrected for linear cross-talk and calibrated for each individual measurement with an automated procedure [23].
3 Alpha event characteristics and selection

The spectra of the calibrated core and segment 19 energies, \(E_0\) and \(E_{19}\), are shown in Fig. 8 for a measurement from AST with both \(^{241}\)Am sources irradiating the detector. The signal of the alphas hitting the top and the side of the detector are well separated due to the different structure of the surface layers. The respective backgrounds from natural radioactivity are also shown for comparison.

In this case, electrons or holes are trapped in the crystal and do not reach a contact. After the other charge carriers are collected, the trapped charge carriers still induce signals in the contacts. This results in reduced and unequal values of \(E_0\) and \(E_{19}\), depending on the position of the trapping. In non-collecting segments, so-called truncated mirror pulses [14] are observed where the signal does not return to the baseline.

The characteristic pulses from an event with net hole trapping, \(E_{19} < E_0\), are shown in Fig. 9. The collecting segment 19 shows a lower energy than the core and the two segments underneath, segments 9 and 10, show positive truncated mirror pulses indicating net hole trapping. The characteristic pulses from an event with net electron trapping, \(E_0 < E_{19}\), are shown in Fig. 10, where negative truncated mirror pulses are observed in segments 9 and 10.

Due to the feature of truncated mirror pulses, alpha events affected by charge trapping can also appear as so-called multi-segment events even though they are single-site events. Thus, a strict single-segment 19 cut, \(E_0 \approx E_{19}\), cannot be used to filter out events induced by environmental gammas, which are often multi-segment events as the gammas predominantly perform Compton scattering at these energies. However, in contrast to gamma induced events, the energies measured in the other segments should never be larger than \(E_{19}\) for events induced by alphas from the top. Therefore, a softer single-segment 19 cut was defined to filter out gamma events:

\[ E_0 \approx E_{19} \]
Fig. 9 Pulses of a typical event with net hole trapping of the a core and segment 19 and b the two closest segments 9 and 10 of a measurement from RSS at $\phi = 180.6^\circ$ and $r = 18.8\,\text{mm}$. The observed energies, $E_0$ and $E_{10}$, are also indicated. The horizontal line in the inset in a is at the mean of the tail of the core pulse.

- S-cut: $E_{19} > \sum_{i=1}^{18} E_i$.

Alpha events affected by charge trapping feature another characteristic: After the correction for the specific decay of charge in the preamplifiers, pulses from “normal” events have a flat tail, see Fig. 7b. However, it has been shown that the pulses of alpha events on passivated surfaces have positive tail-slopes [13,18] after the preamplifier specific correction using the decay constants $\tau_i^\alpha$. These positive tail-slopes are visible in Figs. 9a and 10a.

The possible physical origins of the non-zero tail slopes of alpha-event pulses are a slow release of trapped charge carriers or a very slow drift of a part of the charge cloud due to a very low mobility near the surface. A positive tail-slope corresponds to a seemingly increased decay constant of the pulse, $\tau_i^\alpha$, in comparison to $\tau_i^\beta$. Thus, alpha events can be identified prior to any pulse processing or cross-talk correction by comparing $\tau_i$ with $\tau_i^\alpha$.

Typical $\tau_i$ distributions for events passing the S-cut are shown in Fig. 11 for a measurement from AST and BG. The $\tau_i$ distributions can be modelled by a superposition of Cauchy functions (C) via the function $T(P_T)$ with the parameters $P_T$

$$P_T = \{\mu^T, \sigma_1^T, A_1^T, A_2^T, \mu_\alpha^T, \sigma_\alpha^T\},$$

$$T(P_T) = A_1^T \cdot C(\mu_1^T, \sigma_1^T) + A_2^T \cdot C(\mu_2^T, \sigma_2^T) + A_\alpha^T \cdot C(\mu_\alpha^T, \sigma_\alpha^T),$$

where $\mu^T, \sigma_1^T, A_1^T$ and $A_2^T$ model the underlying background from “normal” events and $A_\alpha^T, \mu_\alpha^T$ and $\sigma_\alpha^T$ model the second peak which is associated with alpha events. The broadness of the distributions comes from low-energy events, for which the electronic noise is relatively large. Hence, the extracted value for $\tau_0$ can be quite different from $\tau_0^\beta$. Selecting only events above about 1 MeV results in two clearly separated peaks with FWHM of about 1 $\mu$s. However, this would also remove alphas with low energies.

In order to study charge trapping in detail, the events induced by alphas from the top source are selected with the S-cut and a second cut:

- $\tau$-cut: $\tau_0 \in [\mu_{\alpha,0}^T \pm 2\sigma_{\alpha,0}^T]$ and $\tau_{19} \in [\mu_{\alpha,19}^T \pm 2\sigma_{\alpha,19}^T]$.

Figure 12 shows the $E_0$ and $E_{19}$ spectra before the alpha selection cuts, after applying the S-cut and after applying the additional $\tau$-cut (Sr-cut).

The S-cut removes events with alphas entering the side of the detector and suppresses gamma events, for which most of the energy is deposited outside of segment 19. After the Sr-cut, only alpha events on the top remain. Note that the $\tau$-cut is a coincidence cut, requiring that $\tau_0$ and $\tau_{19}$ are both within the respective intervals. Above 1000 keV, they form a broad peak. It has been cross-checked that the events in the energy region of the broad alpha peak indeed form the secondary peak observed in the $\tau$ distribution, confirming that the $\tau$-cut selects alpha events [18]. Similarly, analysing the mirror pulses from the neighbouring segments also shows that the Sr-cut is effective in selecting alpha events with charge trapping. These checks verify that the core pulse alone is sufficient to select alpha events. Thus, the rejection of events based only on positive tail slopes, is confirmed to be an effective way to reduce the background for $0\nu\beta\beta$ decay searches.
Distributions of $\tau_0$ and $\tau_{19}$ for events selected with the S-cut from AST at $\phi = 257.9^\circ$ and $r = 23.8$ mm and from BG. The solid line is the function $T$, see Eq. (2), fitted to the distributions of the $^{241}$Am measurement. The $\pm 2\sigma$ interval, used for the $\tau$-cut, is indicated by the vertical dashed lines.

Spectra of $E_0$ and $E_{19}$ before and after the application of the S-cut and $S\tau$-cut for a measurement of the scan AST with the top beam-spot at ($\phi = 257.9^\circ$, $r = 23.8$ mm) and the side beam-spot at ($\phi = 167.9^\circ$, $z = 40.0$ mm).

Correlation between core and segment 19 energies of alpha events selected as described in Sect. 3 from a measurement of the scan AST at $\phi = 232.9^\circ$ and $r = 23.8$ mm. Also shown are the two marginalisations. The dashed (black) lines mark the position of the parameter $E_{\mu,j}^{0/19}$ for this measurement $j$ of the respective fitted function $M$, see Eq. (4), shown as a solid (red) line.

It should be noted, that signal events very close to the surface might also be rejected.

### 4 Location dependence of charge trapping

The correlation between $E_0$ and $E_{19}$ is shown in Fig. 13 for the selected alpha events from the measurement at $\phi = 257.9^\circ$ and $r = 23.8$ mm from AST. Events at this radial position are subject to more electron trapping and higher energies are observed in segment 19 than in the core. The $E_0$ and $E_{19}$ distributions were fitted above 1000 keV via maximum likelihood estimation to find the most likely $E_0$ and $E_{19}$. The function $M(E|P_M)$, with the parameters $P_M$, defined as

$$P_M = \{A, R, E_\mu, \sigma_1, \Delta E_\mu, \sigma_2, s\},$$

$$M(E|P_M) = A \cdot [(1 - R) \cdot \mathcal{N}(E|E_\mu, \sigma_1) + R \cdot \mathcal{N}(E|E_\mu - \Delta E_\mu, \sigma_2) \cdot \text{erf}(-s \cdot (E - (E_\mu - \Delta E_\mu)))] + 1)$$

was chosen to model the distribution of observed energies of the selected events.

It consists of two Normal distributions $\mathcal{N}$: the first, $\mathcal{N}(E_\mu, \sigma_1)$, modelling the main peak and the second, $\mathcal{N}(E_\mu - \Delta E_\mu, \sigma_2)$ modulated by an error function, modelling the low-energy tail of the distribution. The parameter $E_\mu$ corresponds to the most likely observed energy of the alphas.
The obtained values for the core, $E_{\mu, \phi, \text{obs}}^0$ and segment 19, $E_{\mu, \phi, \text{obs}}^{19}$, for the different measurements in the radial scans RSF (fast axis) and RSS (slow axis) are shown in Fig. 14 as a function of $r$.

The uncertainties on the fitted values of $E_{\mu}$ are only a few keV. These results confirm the trends observed previously [14] that for events at smaller radii hole trapping dominates and moving towards segment 19 electron trapping becomes dominant. This can be understood as a higher probability of charge trapping when the charge carriers have a longer drift path towards the contacts. The result of the two scans reveal a dependence of the amount of charge trapping on the crystal axes orientation. The energies observed in the scan along the fast axis are up to 1 MeV higher than those in the scan along the slow axis.

The fitted values of $E_{\mu, \phi, \text{obs}}^0$ and $E_{\mu, \phi, \text{obs}}^{19}$ over $\phi$ are shown in Fig. 15 for the measurements of the rotational scan AST at $r = 23.8$ mm. There is a clear effect of the crystal axes on $E_{\mu, \phi, \text{obs}}^0$ and $E_{\mu, \phi, \text{obs}}^{19}$.

Near a fast axis, more energy is recorded, which would imply a thinner dead layer or less net trapping of charge carriers. The latter is reasonable as the mobility for drifts along the fast axis is higher. An effect of the crystal axes on the observed alpha energies is seen for the first time in GALATEA. This was possible due to the increased amount of data compared to previous studies [14]. In Fig. 15, there is a jump in $E_{\mu}$ between the two measurements around $\phi = 125^\circ$. Between these two measurements, there was a pause of about one day in the data taking. Thus, these two measurements were probably taken at different crystal temperatures.

The open markers in Fig. 15 show data points taken four months after the original scan. Several warming-cooling cycles probably changed the surface conditions influencing the amount of charge trapping. These changing surface conditions are likely due to build-up of surface charges in the passivation layer as also observed for a p-type point contact (PPC) detector in the same setup [24]. Surface charges would change the local electric field at the surface: either attracting or repelling charge carriers towards or from the surface. Thus, the amount of charge carriers affected by trapping would be changed. However, as the observed amount of charge trapping is much less for Super-Siegfried than for the PPC, surface charges were not included in the simulations presented in this paper. If they were included, also charge-cloud effects should be considered. In order to disentangle the contribution of pure surface effects and surface charges, more measurements are required in which a possible surface charge could be measured, e.g., through a monitored guard ring placed just above the passivation layer.

Comparing $E_{\mu}$ of measurements at about the same location from the scan AST, see Fig. 15, and the rotational scans RSF and RSS, see Fig. 14a and b, reveals a large difference of about 500 keV in $E_{\mu}$. This also indicates a change of surface charges between the scans or a strong dependence of charge trapping on the crystal temperature.

5 Simulation of charge trapping

A dead layer alone can only equally reduce the alpha energy observed in the core and segment 19. It can neither explain the observed differences between $E_{\mu, \phi, \text{obs}}^0$ and $E_{\mu, \phi, \text{obs}}^{19}$ nor the observed truncated mirror pulses in non-collecting segments. The observed alpha energies can only be explained by taking charge trapping effects into account. There is no established microscopic model available which includes charge trapping. Here, a model consisting of three different parts is introduced to describe the radial dependence of $E_{\mu, \phi, \text{obs}}^0$ and $E_{\mu, \phi, \text{obs}}^{19}$. The model was implemented using SolidStateDetectors.jl (SSD) [16], which is an open-source package to simulate solid-state detectors such as germanium detectors. It is written in the Julia programming language and comprises the calculation of the electric field, $\mathbf{E}$, the weighting potentials [16, 25] of the contacts, $W_i$, the drift of the charge carriers through the semiconductor and the induced signals on the contacts. The drift of the charge carriers is calculated in time steps by deriving a drift vector, $v_d$, from the mobility, $\mu e/h$, and the electric field at the current position of the respective charge carrier: $v_{d}=\mu e/h \cdot \mathbf{E}$. In each time step, the signal in each channel is determined by evaluating the weighting potential of all charge carriers at their current position.

The three parts of the model describing the physics underneath the passivated surface are:
1. a so-called dead layer,
2. a so-called surface channel,
3. probabilistic charge trapping.

The dead layer varying with $r$, $DL(r)$, is implemented for a thickness modelled as a quadratic function with three parameters, $DL_1$, $DL_2$ and $DL_3$, which are the dead-layer thicknesses at the radii 12.8 mm, 23.0 mm and 34.8 mm. The allowed parameter space for these three parameters was chosen as $[0, 20] \mu$m which is motivated by the location of the Bragg peak for alphas as described in Sect. 2. For all $r$, $DL(r)$ is forced to be $\geq 0 \mu$m. The initial energy, $Q_{\text{init}}^*(r)$, of the

\[1\] The temperature close to the detector is monitored in GALATEA, but was not stored long term.

\[2\] The manufacturer is, however, extremely reluctant to bid for such a detector.
events is the reduced energy based on the thickness of the dead layer at the respective radial position. The reduction is calculated by integrating the energy loss of alphas in germanium over the dead-layer thickness [18].

The surface channel is implemented in the simulation as a virtual volume, in which \( \mathbf{v}^{e/h}_{d,m} \) is modulated to ensure a drift parallel to the passivated top surface,

\[
\mathbf{v}^{e/h}_{d,m} = (\mathbf{v}^{e/h}_{d} \cdot \mathbf{e}_r) \cdot \mathbf{e}_r + (\mathbf{v}^{e/h}_{d} \cdot \mathbf{e}_\varphi) \cdot \mathbf{e}_\varphi,
\]

where \( \mathbf{e}_r \) and \( \mathbf{e}_\varphi \) are the radial and azimuthal unit vectors. This virtual volume is a tube directly underneath the top surface with a height of 100 \( \mu \)m, ranging from \( r = 10.05 \) mm to \( r = 37.45 \) mm. The height of the virtual volume is motivated by the fact that charge trapping was not observed for 59.5 keV gammas also emitted by the \( ^{241}\text{Am} \) source [18]. Most of these gammas interact with the germanium within about 1 mm. Thus, only events very close, \( O(20 \mu m) \), to the surface seem to be affected by surface effects. The modulation of the drift vector, which corresponds to a modulation of the mobility tensor, is justified as the assumption of an infinite crystal made in the derivation of the mobility tensors for electrons and holes is not valid this close to the surface. In addition, the density of crystal imperfections is likely to be higher close to the surface due to the cutting and polishing processes and the passivation process. The already mentioned surface charges might also impact the behaviour of charge carriers very close to the surfaces. Disentangling all these effects, and the depths to which they have to be considered, will be the topic of future studies. Charge-cloud effects will have to be considered in the simulation models. These effects were only recently implemented in SSD and were, thus, were not yet be considered in the simulations for this paper.

It is also clear that the environment of the detector has to be taken into account in the simulation when handling the drift of charge carriers close to surfaces. If the field simulation is limited to the volume of the detector, reflecting boundary conditions are typically used at surfaces like the passivated top plate. This, however, forces the \( z \)-component of the elec-
For the fit, one event per set of parameters was simulated for each location. Each event was simulated with 2000 electron-hole pairs, $N_{ep} = 2000$, and the signal induced by each charge carrier was weighted with $Q_{ep}^*(r)/N_{ep}$. Each of those charge carriers could get trapped in each step of the drift as described earlier. In the fit, the seed for the random numbers was fixed. Thus, the same random numbers were used for each set of parameters and, therefore, each specific set of parameters always resulted in the same simulated energies. It was tested and verified that the large number of charge carriers ensured that the simulated energies of the events were basically independent, $\mathcal{O}(1\text{keV})$, of the chosen seed.

The likelihood, $\mathcal{L}$, that a set of parameters represents the data was calculated using simulated energies, $E_{\mu,j,\text{sim}}^{0/19}$, in the core and segment 19 for events spawned at all measurement positions of the scan RSF. The data are the most likely observed alpha energies, $E_{\mu,j,\text{obs}}^{0/19}$, as shown in Fig. 14a for each position of the scan RSF for the core and segment 19.

The simulation does not take certain systematic effects into account. Therefore, the simulated core and segment 19 energies were associated with an estimated uncertainty of $\sigma_{\text{sim}} = 100\text{keV}$. The individual likelihood, $l_j^{0/19}$, for each core and segment 19 energy at each radial position is calculated as

$$l_j^{0/19} = \mathcal{N}(E_{\mu,j,\text{sim}}^{0/19}, \sigma_{\text{sim}})(E_{\mu,j,\text{obs}}^{0/19})$$

where $\mathcal{N}(E_{\mu,j,\text{sim}}^{0/19}, \sigma_{\text{sim}})$ is a Normal distribution with mean $E_{\mu,j,\text{sim}}^{0/19}$ and a standard deviation of $\sigma_{\text{sim}}$ evaluated at $E_{\mu,j,\text{obs}}^{0/19}$. The overall $\mathcal{L}$ is given as the product over all positions:

$$\mathcal{L} = \prod_j l_j^{0/19}.\quad(8)$$

The result of the fit is shown in Fig. 17. The simulation follows the trend of the data very well. The marginalised posterior distributions of the parameters $DL_1$, $DL_2$ and $DL_3$ are shown in Fig. 18 and of the parameters $p_{t,0}^e$ and $p_{t,0}^h$ in Fig. 19. The fit suggests that the dead-layer thickness increases towards the mantle of the detector reducing the amount of energy deposited in the active volume. The passivation layer, as told by the manufacturer, has a thickness of about 2 $\mu$m. The remaining dead-layer thickness might be due to damages to the crystal caused in the surface processes, leading to a very low, close to zero, mobility such that created electron-hole pairs directly recombine and are, thus, not detected. It also suggests that the trapping probability

$$p_{t,0}^e, p_{t,0}^h \in [0, \infty] \mu m/\text{nsec}^2$$

ensuring $p_{t,0}^e/\Delta t [\mu m] < 0, 1$. In each step, a random number between 0 and 1 is generated. If the generated number is below the $p_{t,0}^e, p_{t,0}^h$ of that step, the charge carrier is permanently stopped (trapped) at its current position.

A Bayesian fit was performed with the software BAT.jl [26] to the data points of RSF to determine the best values for the five parameters $DL_1$, $DL_2$, $DL_3$, $p_{t,0}^e$ and $p_{t,0}^h$. Flat priors were assumed for all five parameters.

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3 E.g. possible inhomogeneities of the crystal and passivation layer, varying temperatures $\mathcal{O}(5\text{K})$ in GALATEA, details of the impurity profile, charge-cloud effects, no (simulated) trapping along the widening of the borehole.

4 The manufacturer expected a much thicker dead layer.
Dead-layer thickness as given by the fit to the data of the scan RSF, see Fig. 14a.

Deposited energy $Q^*$ corresponding to the depth of the dead layer and simulation results in form of $(1\sigma, 2\sigma, 3\sigma)$ posterior-predictive credibility intervals (solid, dashed and dotted lines) for $E_{\mu,j,\text{obs}}^0$ and $E_{\mu,j,\text{obs}}^{19}$ of the scan RSF. The error bars do not show the uncertainty on the data points but $\sigma_{\text{sim}} = 100$ keV.

Marginalised posterior distribution, $p(DL_k)$, of the thickness of the dead layer at $r = 12.8$ mm ($DL_1$), $r = 23.0$ mm ($DL_2$) and $r = 34.8$ mm ($DL_3$).

Marginalised posterior distribution, $p(p_{\ell,0}^{\epsilon/h})$, of the two parameters describing the charge-trapping probability.

is about a factor of three higher for electrons than for holes. Repeating the same fit for RSS leads to the same conclusion. The model could also be extended such that an azimuthal dependence is modelled and a combined fit to all three scans RSF, RSS and AST could be performed. However, as there are still many uncertainties due to possible surface charges, this was not done. In addition, charge-cloud effects and a non-zero sized beam-spot should be considered in the simulations before performing such a combined fit.

The parameters of the global mode of the fit were used to simulate 10,000 events at each radial position of the scan RSF. Each event was simulated with $N_{ep} = 30$ and no seed was set. The distributions of $E_{\mu,j,\text{sim}}^0$ and $E_{\mu,j,\text{sim}}^{19}$ and measured $E_{\text{data}}^0$ and $E_{\text{data}}^{19}$ are shown in Fig. 20 for the three radial positions 14.8 mm, 24.8 mm and 34.8 mm. Different values for $N_{cp}$ were tried and $N_{cp} = 30$ was found to produce as broad energy distribution like seen in the data due to statistical fluctuations. The relatively low value of $N_{cp} = 30$ resulting in reasonably broad distributions could mean that the trapping mechanism actually happens in some coherent way, such that always a group of electrons or holes gets trapped during the drift. Another explanation might be that there are certain locations at the surface where charge carriers are more likely to get trapped such that, again, a group of electrons or holes is trapped at the same time or, respectively, at the same location.

Even though the model was not tuned to predict correlations, correlations similar to the observed correlations are produced. For events at lower and larger radii, see Fig. 20a and c, the measured 2D-distributions are narrow and stretched. This is also predicted by the simulation, see Fig. 20d and f. It can be explained by the shapes of the weighting potentials of the contacts, see Fig. 21. The gradient of the weighting potential increases close to the respective contact.

For events at larger radii, the holes have only a short drift path towards segment 19 and, thus, less holes are trapped during the drift. In addition, trapped holes still contribute significantly to the segment 19 signal as they are close to the contact. The electrons, however, are trapped at lower radii where the gradient of the weighting potential of segment 19 is basically zero. Thus, the exact location of the trapping of electrons does not influence the signal of segment 19 after the electrons moved inwards below a certain radial position, where the weighting potential of segment 19 is almost constant. Therefore, for events at small (large) radii the spread of $E_{19}$ ($E_{0}$) for a given $E_0$ ($E_{19}$) is larger than the spread of $E_0$ ($E_{19}$) for a given $E_{19}$ ($E_0$).

The simulated 2D-distributions at $r = 14.8$ mm and $r = 34.8$ mm, see Fig. 20d and f, seem not to be as parallel to the diagonal line, $E_0 = E_{19}$, as the measured 2D-
Fig. 20 Correlation between core and segment 19 energies and their marginalisations next to them. On the left a–c: alpha events selected as described in Sect. 3 of three measurements from RSF. On the right d–f: simulated alpha events spawned at the position of the respective measurement shown on the left. The histograms obtained from the simulations are scaled to the respective histogram on the left.
distributions, see Fig. 20a and c. However, this is probably because the spread of the beam-spot was not taken into account in the simulation. All simulated events were spawned at the center of the beam-spot. Taking the spread of the beam-spot into account, see Fig. 6, would result in a superposition of the distributions for the different \( r \) in the beam-spot. This is probably also the reason why the simulation does not produce a half-moon shaped distribution at \( r = 24.8 \) mm, see Fig. 20e, as observed in the data, see Fig. 20b.

The simulation does not include the low-energy tails in the data which are due to collimation effects, see Fig. 5. It produces normally shaped distributions for \( E_0 \) and \( E_{19} \), see Fig. 20d–f. It is, however, interesting that the low-energy alphas seem to be affected by charge trapping in the same way as the high-energy alphas. The trapping mechanisms seem to depend only on the location and not on the total energy deposited.

6 Effect of metalisation

In previous studies \([14]\), a strong dependence of the rise time of the pulses on \( \varphi \) was observed for both alpha and gamma induced events in segment 19. For these studies, segment 19 was only metalised in a small area where the read-out cable was, and is, connected to the segment at \( \varphi_{io} = 135^\circ \) over a range of about 20\(^\circ\). Since then, the detector was reprocessed and segment 19 became fully metalised.

The rise time, \( T_{90}^{10} \), defined as the time in which the pulse rises from 10 to 90% of its maximum amplitude, is used for the rise-time studies presented here. The distribution of \( T_{10}^{90} \) of the core and segment 19 pulses of alpha induced events is shown in Fig. 22 for one position of the scan AST. The histograms were fitted with scaled Normal distributions for each position. The fitted means of these distributions as a function of \( \varphi \) are shown in Fig. 23 for both the core and segment 19.

The core pulses show the expected modulation due to the crystal axes and a small dependence on \( \Delta \varphi_j = |\varphi_j - \varphi_{io}| \), where \( \varphi_j \) is the azimuthal position of the measurement \( j \). This is quantified by comparing the rise times at two positions close to different fast axes of the crystal. At positions close to the fast axis at \( \varphi \approx 225^\circ \), the rise time \( T_{10}^{90} \) is about 15 ns longer than at positions close to the fast axis near \( \varphi_{io} \).

For segment 19, the effect due to the distance to the readout, \( \Delta \varphi_j \), is much stronger than the influence of the crystal axes, which becomes less observable. Here, \( T_{10}^{90} \) is about 205 ns at \( \varphi \approx 225^\circ \) and only about 135 ns at \( \varphi_{io} \). This difference of about 70 ns is, however, strongly reduced compared to the previous measurements \([14]\), where a variation of the rise times of about 730 ns in segment 19 and about 50 ns in the core was observed.

It should be noted, that the position of the axes were determined with events induced by alphas from the side of the scan AST \([18]\). There, the effect due to the crystal axes on \( T_{10}^{90} \) is much more pronounced and not superimposed with the large effect due to the contacting scheme of segment 19 as segments 4, 13, 14 and 15 were the collecting segments, see Fig. 3a.

The dependence of \( T_{10}^{90} \) on \( \Delta \varphi_j \) is not only present for alpha induced events on the top surface but also for events induced on the top by 59.5 keV gammas emitted from the Americium source \([18]\).

Prior to full metalisation, not only the rise times of events induced from the top were, but also events induced from 121.8 keV gammas,\(^5\) entering segment 19 from the side of the detector from a \(^{152}\)Eu, were affected. The values of \( T_{10}^{90} \) for segment 19 showed a very strong dependence on \( \Delta \varphi_j \) \([14,27]\) as shown in Fig. 24a. No such effect was observed for core pulses, see Fig. 24b.

\(^5\) Alpha events could not be induced on the side of segment 19 because it was, and is, covered with Kapton tape.
Fig. 23  Fitted means of the distribution of $T_{90}^{10}$ for the core and segment 19 of events induced by alphas from AST. The error bars indicate systematic uncertainties due to the slightly fluctuating temperature of the detector in GALATEA [23].

Fig. 24  Averaged rise times $T_{90}^{10}$ of events induced by collimated 121.8 keV gammas from $^{152}$Eu entering segment 19 from the side for a segment 19 and b the core before full metalisation, adapted from [14,27]. The $\varphi$-axes were modified to match the coordinate system chosen for this paper. c Rise times $T_{90}^{10}$ determined from the superpulses formed from the gamma events induced by 59.5 keV gammas from the $^{241}$Am source from the rotational side scan ASS after full metalisation. The error bars indicate systematic uncertainties due to the slightly fluctuating temperature of the detector in GALATEA [23].
The extremely long rise times could be explained by a non-zero resistance of the non-metalised over-doped $p^+$ layer. Thus, the depleted volume and undepleted volume in an electronic schematic of a two-channel detector would need to be modelled as two components in series: The depleted volume would still act as simple capacitor but the undepleted volume would need to be modelled as a capacitor and a resistor in parallel. This RC component would lead to longer pulses for segment 19. This was calculated for one-dimensional systems [28].

After the full metalisation, only a very small dependence of $T_{10}^{90}$ on $\Delta \varphi_j$ is observable as shown in Fig. 24c where the rise times of superpulses$^6$ [18] of 59.5 keV gamma events from the scan ASS are depicted. In contrast to the previous measurements, the modulation reflecting the crystal axes is now also visible in segment 19. This indicates that details of contacting and metalisation can influence pulse shapes significantly. Such considerations could help to design germanium detectors such that events close to passivated surfaces could be easily identified. One idea is to leave a gap between the passivation and the beginning of the metalisation. Charge carriers of events close to the passivated surface would drift towards this non-metalised gap resulting in longer rise times compared to events from the bulk, which would directly drift to the metalised regions of the contact.

7 Summary and outlook

Charge trapping was observed in alpha events on the passivated surface of the end-plate of an n-type true-coaxial segmented HPGe detector. Such events occur with energies in the region around 2 MeV where the signal for $0\nu\beta\beta$ decay in $^{76}$Ge would appear. The trapping of holes and electrons was clearly identified by truncated mirror pulses observed on the segmented mantle of the detector. This identification confirmed previous studies from MAJORANA DEMONSTRATOR, that alpha events can be selected effectively by analysing the tail slope of the core pulses. Thus, the background due to alphas on the passivated surfaces can be efficiently suppressed for detectors as used in the first phase of the LEGEND experiment currently under construction at the Gran Sasso underground laboratory.

Radial scans of the detector top surface showed that charge trapping is dominated by hole trapping for events at small radii and by electron trapping for events at large radii as expected from the length of the respective drift paths. The trapping probability per $\mu m/\text{ns}^2$ was found to be three times larger for electrons than for holes for drifts directly underneath the passivated top surface. A dependence of the probability of charge trapping on the crystal axes has been observed for the first time in GALATEA. Near a fast axis, (100), less net charge trapping is observed than near a slow axis, (110). This could be connected to the higher mobilities along the fast axis.

Charge trapping was simulated with the open-source software package SolidStateDetectors.jl. The radial dependence of the probability of charge trapping can be described by a model including a radius-dependent dead layer, a modulation of the charge-carrier mobility and probabilistic charge trapping of electrons and holes. In the future, the model can be extended to take crystal axes effects into account in order to describe the azimuthal dependence. In addition, new versions of SolidStateDetectors.jl can take charge-cloud effects like diffusion and self-repulsion into account. Furthermore, the non-zero tail slope, used to identify surface alpha events, could be added to the simulation by introducing a probabilistic release of trapped charge carriers in each step similar to the trapping probability, or by letting the trapped charge carriers still drift with a very low velocity.

The influence of the segment metalisation on the pulse shapes of events close to the passivated top surface of the detector was studied. In previous studies, very long pulses were observed close to the top for a metalisation scheme where only small areas were metalised. For a full metalisation, normal (faster) pulses and a much weaker dependence of the rise times on the event position with respect to the position of the read-out contact were observed. However, a small $\varphi$ dependence beyond the crystal axes modulation was observed even for full metalisation. Metalisation schemes could be used to influence the pulses of surface events to facilitate easier identification of such events.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: The data is not in a self explanatory format which would allow it to become public. In the case of interest, the authors should be contacted.]

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$^6$ Superpulses are the averaged pulses of all selected gamma events of a measurement. They are used at these low energies because the electronic noise is too large to determine $T_{10}^{90}$ for individual pulses.
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