THE EFFECT OF CONTACTS ON ENERGY RESOLUTION OF SiC SEMICONDUCTOR DETECTOR IN ALPHA-PARTICLE SPECTROMETRY

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1. Introduction

SiC semiconductor material is suitable candidate for a good resolution α-spectrometry radiation detector manufacturing. High radiation and temperature resistance of SiC-based detectors compared to conventional semiconductor materials as silicon and germanium, make them advantageous for many applications in harsh environments. Their ability to serve for radiation monitoring e.g. in actinide waste-tank environments or spent nuclear fuel assemblies has been already demonstrated [1, 2].

Potentially excellent resolution of SiC detectors in α-particle spectrometry was recently limited by the technology of detector fabrication. As their active volumes that could be prepared were thinner than the range of alpha particles of energies of several MeV, the impinging particles were not able to deposit the whole carried energy and thus satisfyingly contribute to the output electric signal.

At present, SiC Schottky diodes with 100 μm thick epitaxial layer overcame this limitation and detectors achieving full width at half maximum (FWHM) better than 20 keV (@ ca 5 MeV) are available [2, 3].

There are several contributing items to the whole FWHM, which will be briefly described in this paper. We investigated deeper the major contribution negatively affecting the resolution, which is the energy broadening caused by the contacts. Monte Carlo-based methods, like MCNPX code (Monte Carlo N-Particle eXtended, [4]), TRIM (Transport of Ions in Matter, [5]) and S3M (SRIM Supporting Software, [6]) have been used to calculate the limiting α-particle resolution caused by the contacts. The relation between simulation and experimentally obtained results will be also discussed.

2. Energy resolution and its limiting factors

When α-particles enter the active volume of a SiC detector, primary collisions of the incident particles with both the atomic electrons (ionization) and the silicon and carbon nuclei (scattering) occur. They are followed by a cascade of impact-ionization events, in which electron-hole pairs are generated and account for an output electric signal.

In the case of SiC-based detectors, there are two main fundamental limitations affecting the width and shape of the spectral line. The first can be assigned to *the energy losses in the events of elastic scattering by Si and C atoms*. These scattering events result in shift (~ 10 keV) and broadening of the spectral line, which possess a Gaussian-type distribution with an extended tail in low-energy region. For α-particles impinging SiC detector material is the respective contribution $\mathrm{FWHM}_{\mathrm{nucl}}$ ~ 4.22 keV [7]. The second limitation relates to *ionization fluctuations and noise*. The fluctuations in ionization efficiency are caused by the fact that the electrons created by α-particles lose their energy not only on ionisation but also on excitation of the lattice vibrations, whereby the portion of spent energy is statistically distributed between these two mechanisms. The statistical broadening component can be estimated from the known equation:

$$FWHM_{ion} = 2.35(F\varepsilon_0 E_\alpha)^{1/2}; \qquad (1)$$

where F is the Fano factor, ε_0 is the average energy required for formation of an electron-hole pair and E_α is the α-particle energy. Assuming $F = 0.12$ and $\varepsilon = 7.78$ eV for SiC, we obtain for $E_\alpha = 5.5$ MeV the contribution of $\mathrm{FWHM}_{\mathrm{ion}} \sim 5.3$ keV. The electronic noise broadening component can be determined from the test-pulse width. If we take into account a noise variance $\sigma_{\mathrm{noise}} = 1.7$ keV (~ 4 keV of FWHM) reported by Strokan, *et al.* [7], we obtain the inherent value of the SiC peak broadening of 7.9 keV.

At present, the best achieved energy resolution is, however, at least two times higher. This difference can be attributed to other sources affecting the line width, like leakage current fluctuations, self-absorption in thicker α-sources, detector contacts and entrance window, etc. It has been shown that broadening due to the first item represent a negligible contribution to the total FWHM measured. Thus, the most important role on the discrepancy between the calculated and measured values of the energy resolution seems to be played by detector contacts and a radiation source.

3. Calculation details

To inspect the influence of entrance window on α-spectrometry energy resolution, 4H-SiC Schottky diodes with Au/Ni thin (9/6 nm) and thicker (80/40 nm) blocking contacts were proposed. The MCNPX code and SRIM/TRIM program were used to simulate the transport of α-particles through contact layers. A standard TRIM Monte Carlo simulation uses a point-like mono-energetic source without taking into account real source parameters and source-to-detector geometry. Ruddy, et al. [1] calculated using TRIM FWHMs resulting from range struggling caused by the window greater than the measured total peak width, indicating that the calculated values are incorrect. Hence, to verify the calculations from TRIM we have employed also MCNPX code, where the geometry of the source and detector arrangement can be precisely modelled. In MCNPX simulations, ^{239}Pu^{241}Am^{244}Cm source was represented as a disk source with a diameter of 7 mm placed parallel to and 3 mm far from the circular Schottky contact of a diameter of 0.9 mm. The outside medium was vacuum. We assumed a source emitting mono-energetic α-particles to follow the contribution to the line shift and its broadening caused only by contact materials. The energies of α-particles emitted by the source and their abundances are as follows: ^{239}Pu - 5156 keV (73 %), 5144 keV (15 %) and 5106 keV (12 %), ^{241}Am - 5486 keV (85 %), 5443 keV (13 %), 5389 keV (1.5 %) and 5544 keV (0.5 %) and ^{244}Cm - 5806 keV (77 %) and 5763 keV (23 %). The ranges of α-particles in Au, Ni and SiC calculated using SRIM are for the highest α-particle energy of 5806 keV 10.2 μm, 11.32 μm and 19.82 μm, respectively.

The outputs from the MCNPX code were processed using Origin program to determine the FWHM value from the f2 tally, which provides information on flux density distribution of α-particles escaping the contact layers and entering the active volume of a detector. Results from TRIM program were analyzed using a statistical module of the S3M program, which processes the TRANSMIT.TXT file from the TRIM program and enables to analyze various beam-parameters like energy-distribution, position-distribution (beam-profile), angular-distribution, momentum-distribution, etc. [6].

4. Results

Fig. 1 demonstrates shift and broadening of the ^{241}Am α-particle energy of 5.486 MeV due to range straggling effects in thin (9/6 nm) and thick (80/40 nm) Au/Ni detector window layers.

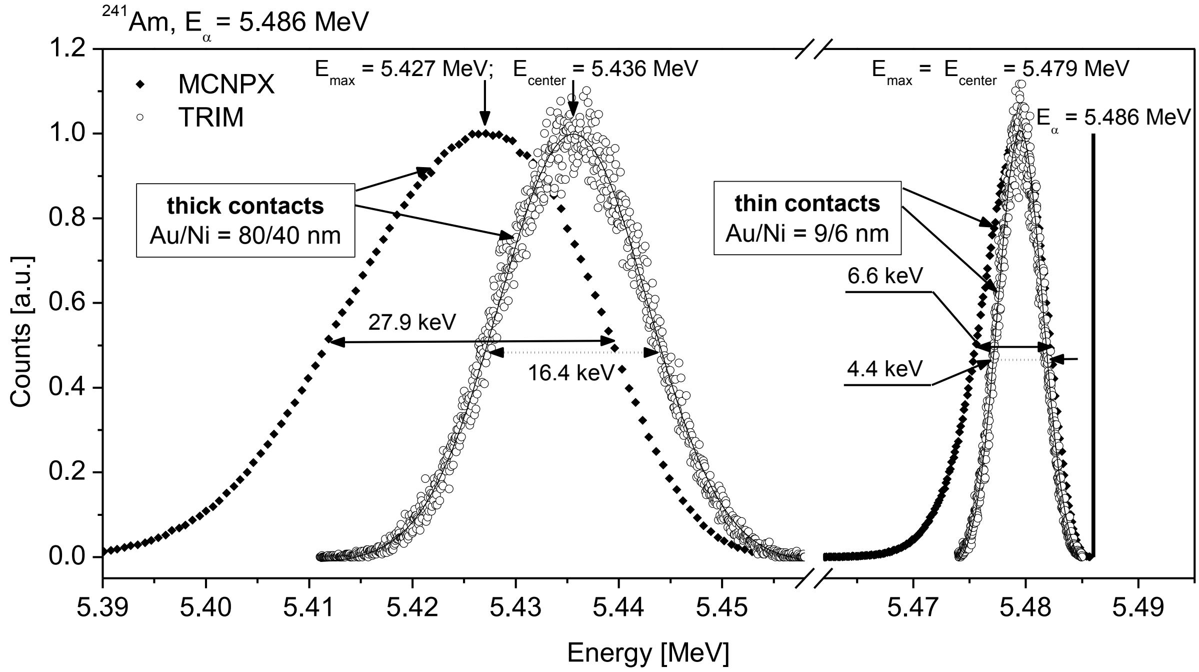

Fig. 1: *A histogram of 5.468 MeV-α-particle energies after passing the thin and thick Au/Ni detector contacts derived from calculations using the MCNPX code (full symbols) and the TRIM program (empty symbols).*

Tab. 1. *Shifts (ΔE) and broadenings (FWHM – full width at half maximum) of the main α-particle energies from the ^{239}Pu^{241}Am^{244}Cm source resulting from energy straggling in the thin and thick Au/Ni entrance layers. Results from MCNPX and TRIM simulations are listed.*

		MCNPX					TRIM + S3M			
Isotope	E_α [keV]	E_{max} [keV]	ΔE [keV]	FWHM [keV]	$FWHM_{left}$ [keV]	$FWHM_{right}$ [keV]	E_{center} [keV]	ΔE [keV]	σ [keV]	FWHM [keV]
thin contacts Au/Ni=9/6 nm										
^{239}Pu	5156	5149.0	7.0	6.71	3.78	2.93	5149.5	6.5	1.77	4.16
^{241}Am	5486	5479.4	6.6	6.61	3.83	2.78	5479.7	6.3	1.85	4.36
^{244}Cm	5806	5799.8	6.2	6.61	3.91	2.70	5799.9	6.1	2.32	5.46
thick contacts Au/Ni=80/40 nm										
^{239}Pu	5156	5094.9	61.1	28.70	16.16	12.53	5104.0	52.0	6.80	16.00
^{241}Am	5486	5427.1	58.9	27.91	15.50	12.41	5435.6	50.4	6.96	16.38
^{244}Cm	5806	5749.5	56.5	26.98	14.88	12.10	5757.1	48.9	6.87	16.18

The distribution of the α-particle energies on the entrance to the active volume of the detector acquired using MCNPX simulations is represented by full symbols. As can be seen from Fig. 1, the energies of α-particles escaping the contact layers are distributed according to a function possessing an asymmetric shape with elongated low-energy region and mean value shifted with respect to the energy of the incident α-particles. The values of shifts (ΔE) and line broadenings (FWHMs) are listed in Tab. 1 for all main spectral line energies of the ^{239}Pu^{241}Am^{244}Cm source. The values of the observed peak centroid shifts calculated using MCNPX are of about 6 ÷ 7 keV and 57 ÷ 61 keV for thin and thick contacts, respectively; and the corresponding FWHMs are of the order of 7 keV and and 27 ÷ 29 keV.

The resultant energy distributions of transmitted α-particles obtained from TRIM simulations and processed using S3M program are plotted in Fig. 1 by empty symbols. As obvious, a Gaussian function fits well the data from simulation and values of shifts and FWHMs (listed in Tab. 1) are as follows: ΔE ~ 6 keV, FWHM ~ 4 ÷ 5 keV for thin contacts and ΔE ~ 49 ÷ 52 keV and FWHM ~ 16 keV for thick Au/Ni contacts.

The differences between calculations performed by the MCNPX code and TRIM program can be observed in line shifts as well as in distribution shape and its broadening; and are significant especially in case of thick contacts. The asymmetric shape of the energy distribution with extended tail on the low-energy side obtained from MCNPX simulations fits better with measured resultant line shape and can be related to the fact, that α-particles emitted by the source modelled in MCNPX enter the contact material under different angles and accordingly, their paths in the contact layers are of different lengths. Consequently, the energy losses in scattering events are also higher, as compared to mono-directional source assumed by TRIM program. To support this explanation, the simulations using MCNPX code has been performed for the same source conditions as used in TRIM calculations and a good agreement in transmitted α-particle energy distributions has been confirmed.

The poorer statistics of the TRIM data displayed in Fig. 1 as compared to MCNPX simulations is due to the number of histories calculated, which was 99 999 for the TRIM simulations and as high as 1.10^9 using the MCNPX code.

5. Comparison with experimentally obtained values of FWHM

4H-SiC Schottky diodes with thin Au/Ni 9/6 nm Schottky barrier contact were fabricated [3]. The charge collection efficiency close to 100 % at reverse bias exceeding 50 V was determined. The best energy resolution of 13.8 keV (0.25 %) FWHM was observed for the main ^{241}Am alpha energy of 5486 keV at a reverse bias of 200 V [3].

Tab. 2: Comparison of calculated (MCNPX and TRIM) and measured widths (FWHMs) and shifts (ΔE) of the spectral lines for thin Au/Ni Schottky contact SiC detector assuming the value of an electronic noise broadening of 6.5 keV.

Isotope	E_α [keV]	FWHM [keV]		
		MCNPX	TRIM	Experiment
^{239}Pu	5156	11.47	10.20	17.6
^{241}Am	5486	11.50	10.37	13.8
^{244}Cm	5806	11.57	10.95	14.5

The resultant FWHM is comprised of several contributions as discussed above, which can be combined in squares presuming the Gaussian shape of their distributions. If we neglect that α-particles entering the active volume of the detector posses a spectrum deflected from the normal distribution function (as regards the MCNPX calculation), the resultant FWHM comprising the contribution from thin contact straggling effect will be as high as 11.50 keV and 10.37 keV, derived according to MCNPX and TRIM simulations, respectively, for the ^{241}Am peak (Tab. 1). In this calculation we assumed the contribution from the noise of the readout electronic measured using a precise pulsar generator of 6.5 keV of FWHM [3]. As obvious, results from MCNPX simulations are closer to the measured FWHM as those from

TRIM simulations. The difference between measured and calculated values can be attributed to additional line broadening due to self-absorption in the radiation source of the finite thickness or to imperfect collection of the charge carries in the active volume of the detector. Moreover, the value of measured FWHM for ^{239}Pu spectral line can be markedly overestimated due to overlapping with adjacent energy line (5144 keV), which is shifted with respect to the most intense 5156-keV line by only 12 keV.

6. Conclusion

MCNPX and TRIM Monte Carlo programs were used to calculate the contribution to the total line broadening caused by loss of α-particle energy in Au/Ni Schottky blocking contacts of a SiC detector. The results showed that the detector window design influences the measured resultant line width significantly. The values of FWHMs calculated using MCNPX code were about two times higher compared to results from TRIM simulations due to different source and source-to-detector geometry. The total line width comprising the inherent line broadening for SiC was calculated and compared with experimentally obtained values for the case of thin contacts. The observed differences depend on the energy of the α-particle spectral line evaluated and result likely from other contributing factors to line broadening which are not predictable and therefore were not accounted for in our calculations (effect of the radiation source thickness, non-ideality of the SiC detector material in the sense of charge collecting, etc.).

The calculations combined with experimental results showed that SiC material has a great potential to serve for α-spectrometry as a detector with excellent resolution when the entrance window is designed carefully.

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