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Silicon Carbide Neutron Detector Development – Computational Support with MCNP

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ABSTRACT

The development of neutron detectors based on semiconductor technology is increasing due to shortages of ^{3}He in the world. Under project E-SiCure, radiation-hard silicon carbide detectors with neutron converters have been developed and first tests were performed at Jožef Stefan Institute TRIGA Mark II research reactor. The development of silicon carbide detectors is still ongoing and the computational support contributes to the development process an opportunity to test different new configurations. In this paper, the computational support for finding new converter materials for silicon carbide detectors is presented. The analysis is comprised of calculations of reaction rates for all possible isotopes and reactions producing charged particles in the neutron spectra of the TRIGA research reactor. The analysis has provided new possible isotopes to be used as converter materials in addition to the well known ^{3}He, ^{6}Li and ^{10}B. These isotopes are ^{22}Na for detection of thermal neutrons and ^{40}Ca, ^{58}Ni, ^{39}K, ^{35}Cl and ^{33}S for detection of fast neutrons. The most promising isotope is ^{22}Na due to higher (n,p) reaction rate compared to the ^{3}He isotope, which is the commonly used neutron detections material. Additionally, computational support to the development of the silicon carbide detector was provided by the construction of a detailed Monte Carlo model of the silicon carbide detector. The constructed model allows for the calculation of the charged particle spectra in the detector crystal, which can be used for preliminary analysis of new detector designs and materials.

1 INTRODUCTION

Complex geopolitical instabilities and decentralized terrorism threats have lead to the urge to deploy nuclear screening systems for detection of illicit trafficking of nuclear materials.

Neutron detection is an integral part of these detection systems for prevention of trafficking of nuclear materials such as ^{233}U, ^{235}U and ^{239}Pu [1]. Shortages of ^{3}He have caused increased research in the field of new neutron detectors [2, 3]. One of the new neutron detector types under development is the semiconductor silicon carbide (SiC) detector. The E-SiCure project (Engineering Silicon Carbide for Border and Port Security), funded by the NATO Science for Peace and Security Programme, was focused on developing radiation-hard silicon carbide detectors with neutron converters [4]. The developed SiC detector concept was comprised of a neutron to charge particle converter made from ^{6}LiF or $^{10}B_4C$, due to high reaction rate for production of alpha particles and SiC crystal for detection of the generated charged particles. Both detector and neutron converter are located inside a vacuum chamber to reduce the absorption of emitted charged particles in the air. The developed detector has already been tested at the Jožef Stefan Institute (JSI) TRIGA Mark II research reactor, showing promising results for neutron detection [5, 6].

Computational support is of essential importance for the development of detectors as it allows the testing of different concepts before experimental testing. In this paper, calculations to support further development of the SiC neutron detector will be presented. The analysis is comprised of all possible neutron reactions in the ENDF/B-VIII.0 nuclear data library producing charged particles based on the neutron spectra of the JSI TRIGA research reactor [7]. The analysis aims to find new candidate reactions, or isotopes with high reaction rates, which could be used beside the reactions on ^{6}Li and ^{10}B in the neutron converter material and can be experimentally tested at the JSI TRIGA research reactor. Additionally, the analysis also focuses on finding reactions sensitive to fast neutrons as the reactions on ^{6}Li and ^{10}B are triggered predominantly by thermal neutrons.

The computational support for the development of the SiC detectors also consists of charged particle transport in the SiC detector itself with the Monte Carlo N-Particle transport code (MCNP [8]). The aim is to calculate the detector response to charged particles for different neutron converter materials in support of experiments. For this a detailed model of the SiC detector was made in MCNP, taking into account the detailed SiC detector construction [9].

The paper is organized as follows. In section 2 the search for new neutron to charge particle converter materials analysis will be presented. The analysis is comprised of calculations of reaction rates for all possible reactions producing charge particles for all isotopes present in the ENDF/B-VIII.0 nuclear data library in the neutron spectra of the JSI TRIGA research reactor. In section 3 the detailed MCNP model of the 4H hexagonal phase SiC detector (4H-SiC [9]) developed in the E-SiCure project will be presented together with first computational results.

2 NEUTRON TO CHARGED PARTICLE CONVERTER

The isotopes ^{6}Li and ^{10}B are the two commonly used isotopes for converting neutrons into charge particles via reactions $^{6}Li(n,t)\alpha$ and $^{10}B(n,\alpha)^{7}Li$ [5] due to high cross section for reaction with thermal neutrons (energies below 1 eV). Detection of fast neutrons (E above 0.1 MeV) is one of the next steps in the development of the SiC detector. To achieve this, new neutron to charge particle converting materials are needed. Due to this, an analysis was performed to find isotopes with reactions sensitive to fast neutrons that produce charged particles. The analysis was performed with neutron spectra calculated by MCNP using a validated JSI TRIGA Mark II MCNP model [10] and the RR_UNC code for calculations of reaction rates together with uncertainties [11]. At the same time, the analysis also allowed for additional neutron to charge particle isotope materials sensitive to thermal neutrons to be found.

2.1 JSI TRIGA Research Reactor Neutron Spectra

The neutron experimental testing of the developed SiC detector under E-SiCure project was performed in the Dry Chamber of the JSI TRIGA research reactor. The Dry Chamber is a large irradiation room in the concrete body of the reactor, connected with the reactor core by a graphite thermalizing column [12]. To increase the neutron flux and change the shape of neutron spectra in the Dry Chamber, a fission plate was located in front of the SiC detector during experimental measurement. Fig. 1 displays a photograph of the JSI TRIGA reactor and a schematic view of its main components, including the Dry Chamber.

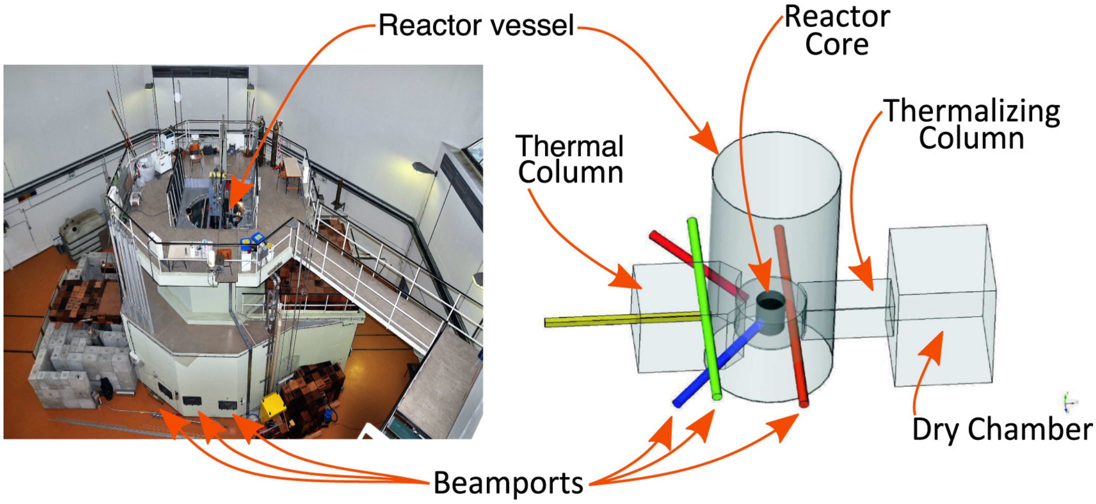

Figure 1: Photograph and schematic view of the JSI TRIGA research reactor. In the figure all main components of the reactor are marked. The figure was taken from [5].

To support the fast neutron detection development of the SiC detector, neutron spectra at the experimental position behind fission plate in the Dry Chamber was calculated with MCNP. Fig. 2 shows the calculated neutron spectra in the Dry chamber used for finding new converter materials for SiC detector.

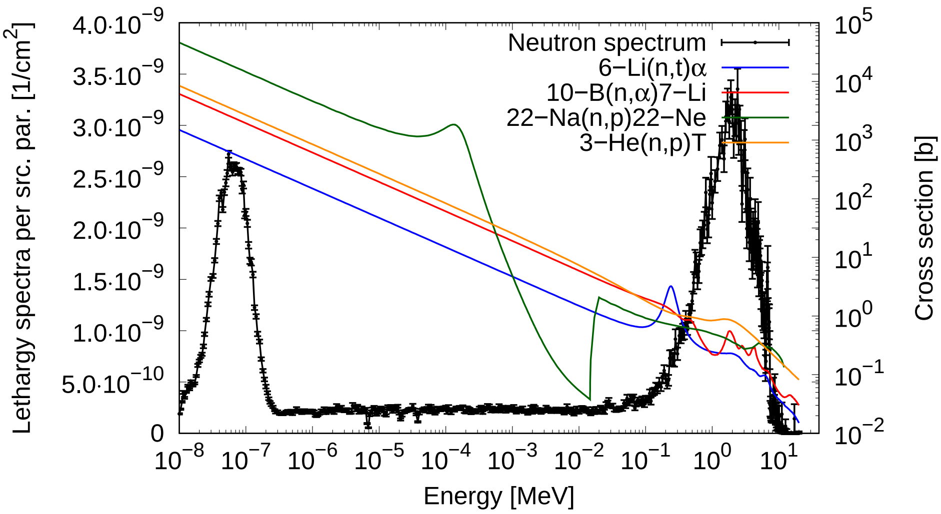

Figure 2: Neutron spectrum used for the search of neutron to charge particle converting materials with the MCNP code. The cross sections for reactions predominantly produced by thermal neutrons are also presented. All cross sections were taken from the ENDF/B-VIII.0 nuclear data library.

2.2 Neutron Converter Analysis

The RR_UNC code was developed at the Reactor Physics department of the Jožef Stefan Institute for calculation of the reaction rates and average cross section [11]. The inputs for the code are neutron spectra and studied cross sections, all in the same energy group structure and ENDF-6 format. For the analysis presented in this paper, the neutron spectra and cross sections were stored in a 640 energy group structure. To take into account all possible isotopes and reactions, the analysis for new converter materials was performed with all isotopes and all reactions in the ENDF/B-VIII.0 nuclear data library [7]. The nuclear data library was chosen as it is the most up to date nuclear data library with 557 isotopes.

The analysis of the reactions rates calculated by RR_UNC focused on reactions (n,p), (n,d), (n,t), (n,^{3}He), (n,α), (n,t2α) and elastic scattering on hydrogen. The highest calculated reactions rates for different isotopes and reactions are presented in Tab. 1. From the results, one new converter material for thermal neutrons was found, i.e. ^{22}Na. Calculated (n,p) reaction rate is higher by an order of magnitude than (n,p) reaction rate for ^{3}He, which is the main isotope for current neutron detectors. This is due to a higher cross section for reaction, which is presented in Fig. 2. Additionally the (n,α) reaction rate of ^{22}Na is also high. However, ^{22}Na is radioactive with a half-life of 2.602 years. Despite this the isotope ^{22}Na is an interesting candidate for neutron converter for SiC detector.

Table 1: Highest calculated reaction rates for different isotopes and neutron to charge particle producing reactions. The E 50 % represents the energy at which the integral of the reaction rate is 50 % of the total reaction rate. The most promising new reactions are marked with grey color.

Isotope	**Reaction**	**Reaction rate per src. par.**	**E 50% [MeV]**	**Natural abundance [%]**	**Radioactive**
H	Elastic scattering	8.98E-05	1.067-7	99.98	stable
22-Na	(n,p)	4.34E-02	4.567-8	traces	2.602 y
3-He	(n,p)	7.99E-03	4.539-8	0.00020	stable
14-N	(n,p)	2.86E-06	4.730-8	99.60	stable
36-Ar	(n,p)	4.66E-07	3.8126	0.3340	stable
40-Ca	(n,p)	3.47E-07	4.48332	96.941	stable
58-Ni	(n,p)	3.45E-07	4.53248	68.077	stable
39-K	(n,p)	3.39E-07	3.46221	93.258	stable
35-Cl	(n,p)	3.24E-07	2.99003	76	stable
54-Fe	(n,p)	2.59E-07	4.71622	5.85	stable
6-Li	(n,t)	1.41E-03	4.543-8	7.59	stable
10-B	(n,α)	5.78E-03	4.540-8	20	stable
33-S	(n,α)	1.13E-06	0.15735	0.75	stable
22-Na	(n,α)	4.41E-05	4.642-8	traces	2.602 y
36-Ar	(n,α)	2.66E-07	3.84933	0.3340	stable
10-B	(n,t2α)	1.49E-07	4.03435	20	stable

In Tab. 1 the energies at which the integral of the reaction rate is 50 % of the total reaction rate are also presented (E 50 %). With this parameter reactions produced predominantly by fast neutrons can be identified. The most promising isotopes are ^{40}Ca, ^{58}Ni, ^{39}K and ^{35}Cl with E 50 % energies in range of several MeV and are solid at room temperatures. Additionally isotopes ^{40}Ca, ^{39}K and ^{35}Cl are often found together in compounds such as $CaCl_2$ and KCl. The (n,α) reaction rate for isotope ^{33}S is higher by an order of magnitude compared to other fast neutron isotopes, but the E 50 % energy is lover at 0.15 MeV. In Fig. 3 cross section for all isotope reactions produced predominantly by fast neutrons are presented. Despite this, all of the isotopes are good candidates for neutron converter for SiC detector.

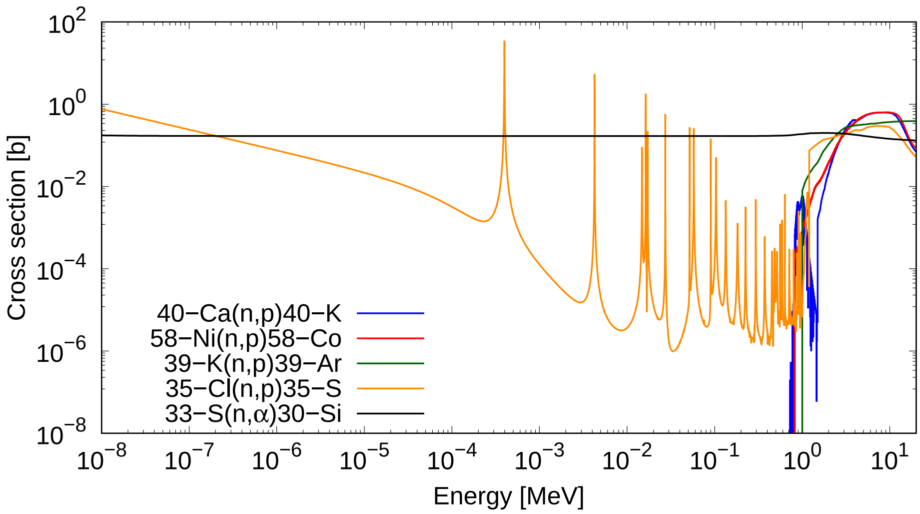

Figure 3: Cross sections for reactions predominantly produced by fast neutrons. All cross sections were taken from the ENDF/B-VIII.0 nuclear data library.

3 SIC DETECTOR MCNP MODEL

The development of SiC detectors can be computationally supported by performing Monte Carlo simulations. This allows new detector designs or new converter materials to be computationally tested before experimental measurements. Due to this, a detailed MCNP model of the SiC detector together with the neutron converter and vacuum vessel components was developed and is presented in Fig. 4. The SiC detector comprises of a $3\ \mathrm{mm} \times 3\ \mathrm{mm} \times 25$ µm epitaxial SiC layer covered by 70 nm thick Ni Schottky contact. The active detector is located at top of the SiC substrate. The SiC substrate has a 70 nm thick Ni contact followed by 0.1 mm Cu Ohmic contact. The whole detector is located on a polycarbonate chip carrier. To support experimental measurements the neutron converter and the vacuum vessel was also modelled. The neutron converter consists of an Al disc on which a thin layer of the neutron converter is applied. The Al disc is glued with adhesive to the polycarbonate cover, which is located around 1 cm from the active part of the SiC detector. The neutron source is located outside the vacuum vessel windows, thus realistically modelling the SiC experimental set-up in the TRIGA Dry Chamber.

3.1 ^{241}Am Response Calculation

To establish the representativeness of the computational model and to verify the computational approach the developed MCNP model of the SiC detector was used to perform MCNP calculations with an ^{241}Am α source as this source was used for the first experimental testing of SiC detector. The transport calculations were performed using the Monte Carlo Neutron Particle transport code MCNP6.2 [8]. In the MCNP calculation, the energy deposition pulse height was tallied in the active SiC volume. The obtained pulse height spectrum from the MCNP calculations matched very well with the experimental measurements presented in Fig. 5.

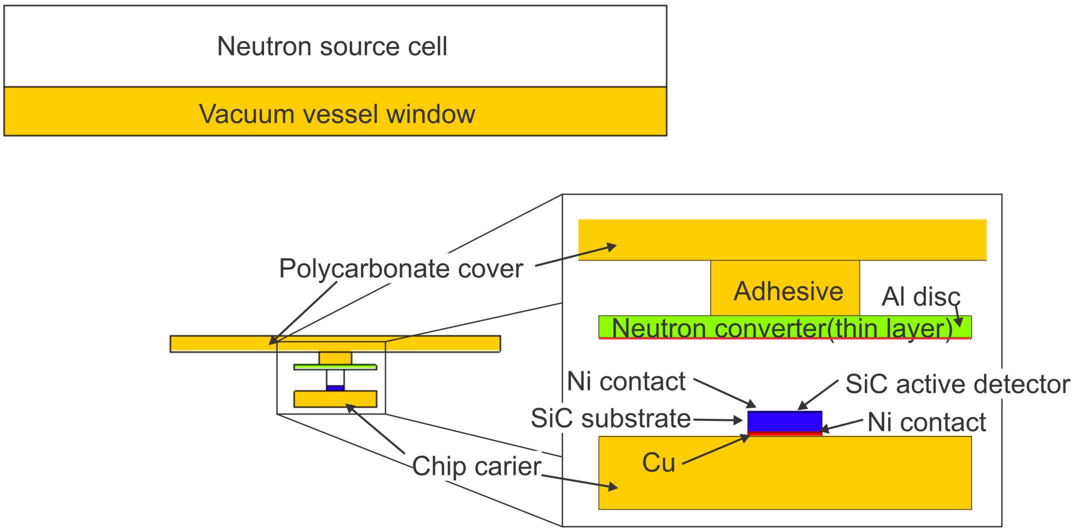

Figure 4: Detailed MCNP model of the SiC detector together with neutron converter. The main structures of the detector vacuum vessel are also modelled for support of experimental measurements.

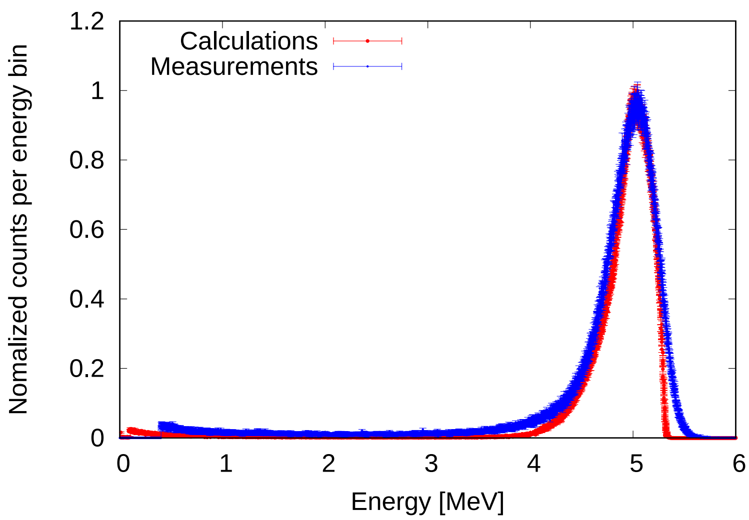

Figure 5: Comparison of measured (blue) and calculated (red) pulse height spectra with an ^{241}Am α particle source.

A critical parameter for the performance of SiC detectors is the thickness of metallic contacts (made in the present case by deposition of Ni) through which the electrical signals are measured and through which the incident charged particles must travel to be detected. As charged particles are slowed down strongly in matter through Coulomb interactions, the best detector performance in terms of resolution and overall efficiency is achieved with thin contact layers. Fig. 6 displays pulse height spectra obtained by variation of the contact layer thickness. Calculations were performed for five values: 50 nm, 70 nm (corresponding to the actual contact layer thickness), 100 nm and 700 nm. It can readily be observed that the calculated pulse height spectra are very similar for the 50 nm - 100 nm contact thickness range, however the pulse height spectrum for the 700 nm contact thickness is strongly shifted towards lower energies, by about 0.5 MeV.

The validated MCNP model of SiC detector will be used in the future support of the SiC

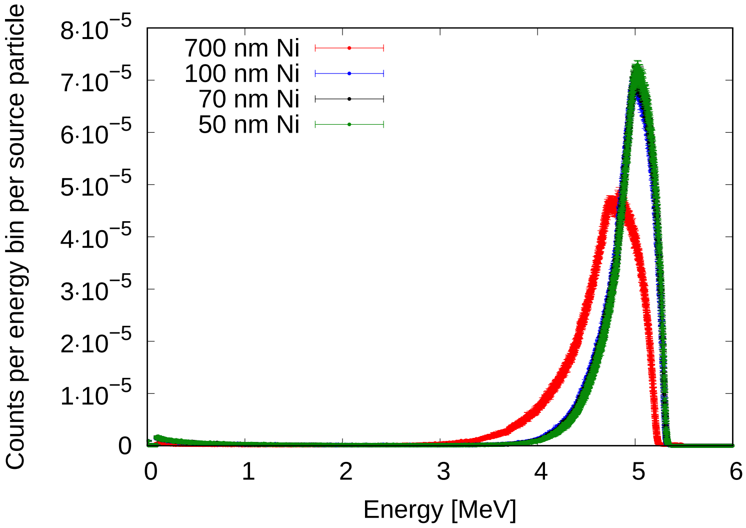

Figure 6: Calculated alpha particle pulse height spectra in SiC for different front Ni contact thicknesses.

detector development. One of the computational support will be testing of SiC detector response for the new neutron to charge particle converter materials found in the research presented in this paper.

4 CONCLUSION

The development of neutron detectors based on semiconductor technology is increasing due to shortages of ^{3}He in the world. Under project E-SiCure radiation-hard silicon carbide detectors with neutron converters have been developed. Computational support is an important tool for the development of detectors as it allows the testing of different concepts before experimental testing. In this paper, computational support for further development of the SiC neutron detector is presented.

The computational analysis performed focused on finding new neutron to charge particle converting materials. The analysis comprised out of the calculation of reaction rates for all possible isotopes and reactions producing charged particles in the neutron spectra of the TRIGA research reactor. The analysis has provided new possible isotopes to be used as converter materials instead of the well known ^{3}He, ^{6}Li and ^{10}B. These isotopes are ^{22}Na for detection of thermal neutrons and ^{40}Ca, ^{58}Ni, ^{39}K, ^{35}Cl and ^{33}S for detection of fast neutrons. The most promising isotope is ^{22}Na due to higher (n,p) reaction rate compared to the ^{3}He isotope despite being a radioactive isotope.

Additionally, computational support to the development of the SiC detector was provided by the construction of a detailed Monte Carlo model of the SiC detector. The constructed model allows for calculation of the charged particle spectra in the detector crystal, which will be used for preliminary analysis of new detector designs and materials in the future development of the detector.

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