

COMPARATIVE STUDY OF THE MeV ION CHANNELING IMPLANTATION INDUCED DAMAGE IN 6H-SiC BY THE ITERATIVE PROCEDURE AND PHENOMENOLOGICAL CSIM COMPUTER CODE

by

Marko P. GLOGINJIĆ^{1*}, Marko V. ERICH¹, Željko V. MRAVIK¹, Branislav VRBAN², Štefan ČERBA², Jakub LÜLEY², Vendula FILOVÁ^{2,3}, Karel KATOVSKÝ³, Ondřej ŠTASTNÝ³, Jiri BURIAN³, and Srdjan M. PETROVIĆ¹

¹ Laboratory of Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

² Institute of Nuclear and Physical Engineering,

Slovak University of Technology in Bratislava, Bratislava, Slovakia

³ Faculty of Electrical Engineering and Communication, Brno University of Technology, Brno, Czech Republic

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Due to its unique material properties, such as extreme hardness and radiation resistance, silicon carbide has been used as an important construction material for environments with extreme conditions, like those present in nuclear reactors. As such, it is constantly exposed to energetic particles (*e. g.*, neutrons) and consequently subjected to gradual crystal lattice degradation. In this article, the 6H-SiC crystal damage has been simulated by the implantation of 4 MeV C³⁺ ions in the (0001) axial direction of a single 6H-SiC crystal to the ion fluences of $1.359 \cdot 10^{15} \text{ cm}^{-2}$, $6.740 \cdot 10^{15} \text{ cm}^{-2}$, and $2.02 \cdot 10^{16} \text{ cm}^{-2}$. These implanted samples were subsequently analyzed by Rutherford and elastic backscattering spectrometry in the channeling orientation (RBS/C & EBS/C) by the usage of 1 MeV protons. Obtained spectra were analyzed by channeling simulation phenomenological computer code (CSIM) to obtain quantitative crystal damage depth profiles. The difference between the positions of damage profile maxima obtained by CSIM code and one simulated with stopping and range of ions in matter (SRIM), a Monte Carlo based computer code focused on ion implantation simulation in random crystal direction only, is about 10 %. Therefore, due to small profile depth shifts, the usage of the iterative procedure for calculating crystal damage depth profiles is proposed. It was shown that profiles obtained by iterative procedure show very good agreement with the ones obtained with CSIM code. Additionally, with the introduction of channeling to random energy loss ratio to depth profile scale conversion, the agreement with CSIM profiles becomes excellent.

Key words: silicon carbide, computer simulation, iterative procedure, RBS/C and EBS/C spectrometry

INTRODUCTION

Rutherford and Elastic Backscattering Spectrometry in the channeling orientation (RBS/C & EBS/C) are ion beam analysis characterization methods that are widely used, among other things, for the investigation of crystal lattice damage [1, 2]. Besides a good sensitivity, simple sample preparation and negligible sample destructiveness, RBS/C & EBS/C are methods with good depth resolution. Namely, in the case of damaged crystal lattice backscattered channeled ions carry additional information about the number of dislocated lattice atoms as well as their crystal depth. Hence, it is possible to obtain quantitative depth

distribution of crystal damage [3]. This is important, especially in the field of nuclear technology, where the interaction of energetic particles with nuclear materials is frequently investigated [4-6].

Damage depth distribution cannot be obtained directly from the RBS/C & EBS/C spectra (in further text BS/C for the channeling and BS for the random mode). To extract that information, several approaches were developed. The first, simpler approach is based on an iterative procedure, which separates backscattering spectra yield which originates due to ion dechanneling process, from the one due to crystal lattice imperfections or damage [7-9]. For the iterative procedure, the BS spectrum of the undamaged crystal represents a completely amorphous structure, while the BS/C spectrum represents a perfect crystal. By recording the BS/C spectrum of the disordered

* Corresponding author, e-mail: marko.gloginjic@vin.bg.ac.rs

crystal and applying the iterative procedure, the damage depth distribution could be obtained. The iterative procedure is widely used for the investigation of damage depth profile only in the near-surface region ($< \sim 1 \text{ }\mu\text{m}$) [10]. This limitation originates from the fact that the energy loss that channeled ions experience is lower than for the non-channeled ones. This difference in energy loss process iterative procedure is not taken into account. However, for the crystal depths close to the surface, the difference in energy loss for channeled and non-channeled ions does not lead to the accumulation of significant error, to hamper the accuracy of iterative procedure.

Damage depth profile can also be extracted from the BS/C spectra using computer codes, most often based on Monte Carlo (MC) simulation method [11]. The MC codes simulate an individual ion interaction with a material, which results in very good accuracy. Despite a good accuracy, calculations based on the MC approach consume a lot of computational time on each spectrum, which could last up to a few hours [10]. Also, the MC calculation sometimes requires initial preconditions, such as dominant defect type, to obtain accurate damage profiles. Recently, in the Laboratory of Physics, Vinča Institute of Nuclear Sciences, CSIM phenomenological code for depth damage profile extraction from BS/C spectra was developed [12]. The procedure is based on the BS/C spectra fitting by assuming the damage depth profile. The process is repeated until the simulated and experimental spectra overlap. In comparison to the MC based codes, the CSIM code is significantly faster, calculating the quantitative crystal damage without the precondition of knowing the types of crystal defects. The maximum investigated depth depends only on the experimental probing particles. It was shown that CSIM provides very good results for the crystal damage depth profile in the case of 4 MeV carbon ion implantation in diamond [13] and 4 MeV carbon and silicon ions implantation in the silicon carbide [3].

Silicon carbide (SiC) is a well-known ceramic material with unique physicochemical properties such as high thermal conductivity, corrosion resistance, excellent all-round mechanical properties, and high radiation resistance [14, 15]. These properties of SiC are the reason for continuous interest in SiC as a material for extreme exposure environments like space [16, 17] and nuclear reactors [18, 19]. Regarding nuclear technology, SiC is used as a structural material in both fission and fusion reactors as cladding materials [20, 21]. Due to constant exposure to the energetic particles (fission products, neutrons, and alpha particles) in reactor environments, degradation of SiC crystal structure occurs. Induced material wear and tear caused by crystal swelling and amorphization, could lead to nuclear accidents. Hence, the investigation of SiC crystal damage and its quantification is contributing to the technological aspect of nuclear materials development.

The neutron damage to the crystal lattice is often simulated by the implantation of self-ions, C or Si ions in our case, usually, to the order of high fluences. Therefore, ion irradiations are often used for the investigation of materials important to nuclear reactor environments [22,

23]. In previous BS/C spectra studies of the 4 MeV C and Si ions channeling implantation in 6H-SiC single crystal irradiated with different fluence, were investigated [3]. The BS/C spectra were probed by the 1.725 MeV and 1.860 MeV protons. Using the CSIM computer code damage depth profiles were calculated. Obtained profiles show very good agreements with the SEM and micro-Raman (R) analysis results, confirming CSIM code efficiency. In this study, additional BS/C spectra of the same 6H-SiC sample implanted by C^{3+} ions in channeling mode were recorded using 1.000 MeV. The 1.000 MeV protons were used as probing particles to avoid dominant resonant nuclear reactions, $^{12}\text{C}(\text{p}, \text{p}_0)^{12}\text{C}$ at 1.731 MeV and the $^{28}\text{Si}(\text{p}, \text{p}_0)^{28}\text{Si}$ at 1.667 MeV, which appear in the case of 1.725 MeV and 1.860 MeV protons. These nuclear resonances significantly influence spectra yield [24]. In this article, we will demonstrate that, in special cases such as this one, iterative procedure obtained crystal damage profiles show very good agreement with the ones obtained by CSIM code, even at a few micrometers of crystal depth.

METHODS AND PROCEDURES

The channeling implantation of carbon ions in the (0001) axial direction of the 6H-SiC single crystal was conducted at Rudjer Bosković Institute, Zagreb, Croatia. For the ion channeling experiment, 1 MV HV Tandem tandem accelerator installation with a collimation system of two apertures with 1 mm in diameter at a distance of 25 cm was used. The crystal alignment with the ion beam was achieved by 1 MeV protons and the five-degree goniometer with an angle accuracy of 0.01° . A proton beam was used for alignment to minimize the crystal lattice damage. The crystal position for the channeling experiment was determined by mapping the ion backscattering yield for different sets of azimuthal and polar angles nearby (0001) crystallographic orientation. The parameter set with the minimum backscattering yield was used for the channeling experiment. The backscattered ions were collected by a surface barrier detector placed at a 160° angle relative to the ion beam direction. During the alignment and implantation procedures, the ion beam current did not exceed 9 nA to avoid overheating the sample. The channeling implantation along the (0001) 6H-SiC crystal direction was conducted using 4 MeV C^{3+} ions. The implantation area was about $1 \text{ mm} \times 1 \text{ mm}$. Fluences applied for each examined sample were presented in tab. 1.

The BS/C analysis was performed with the same experimental set-up as ion channeling implantation. The BS/C spectra were probed by 1 MeV protons. Additional BS/C backscattering yield originating from crystal damage caused by the implanted impurity, in our case self-ion (carbon), is negligible since the implanted concentration is less than 0.5 % (for highest fluence) of crystal atomic concentration. Hence, an in-

Table 1. Channeling experiment parameters – ion type, energy and fluence

Sample	Ion	Energy [MeV]	Ion fluence [cm ⁻²]
S-1	C ³⁺	4	1.359 10 ¹⁵
S-2	C ³⁺	4	6.740 10 ¹⁵
S-3	C ³⁺	4	2.020 10 ¹⁶

crease in BS/C spectra yield of implanted samples compared to pristine samples, can fully be ascribed to damage caused by ion displacement due to passing the energetic particles through the crystal lattice.

THE CSIM CODE

The BS and BS/C experimental spectra are analyzed using the CSIM computer code. The recently developed CSIM computer code is based on the phenomenological approach [12]. The main function of the CSIM code is the extraction of the quantitative damage depth profile from the BS/C spectra. The calculation procedure is based on simulation of the experimental BS/C spectra by adjusting the damage depth profile until a sufficiently good fit of an experimental spectrum is reached. In

order to take into account the spectrum yield originating from the dechanneling process the pristine BS/C spectrum, a χ^2 minimization procedure should be performed. From it the channeling parameters α , the channeling to random stopping ratio, x_c , the dechanneling range, and k , the dechanneling rate are determined. For a more in-depth description of the CSIM computer code, we refer to the study of Gloginjić *et al.* [3].

RESULTS AND DISCUSSION

The 1 MeV proton BS/C spectra of 6H-SiC samples irradiated with 4 MeV C³⁺ ions in (0001) crystal axial direction are presented in fig. 1. All BS/C spectra are normalized according to the collected charge and subsequently fitted using CSIM computer code to obtain damage depth profiles. The BS spectrum of a non-implanted sample (S-rand) is shown in fig. 1(a). Due to the mass difference of Si and C target atoms, a typical two *step* BS spectrum is observed. The surface edge for C atoms is at 0.870 MeV (first *step*), while for Si is at 0.720 MeV (second *step*). The S-rand BS spectrum is fitted both using CSIM (red line) and SIMNRA

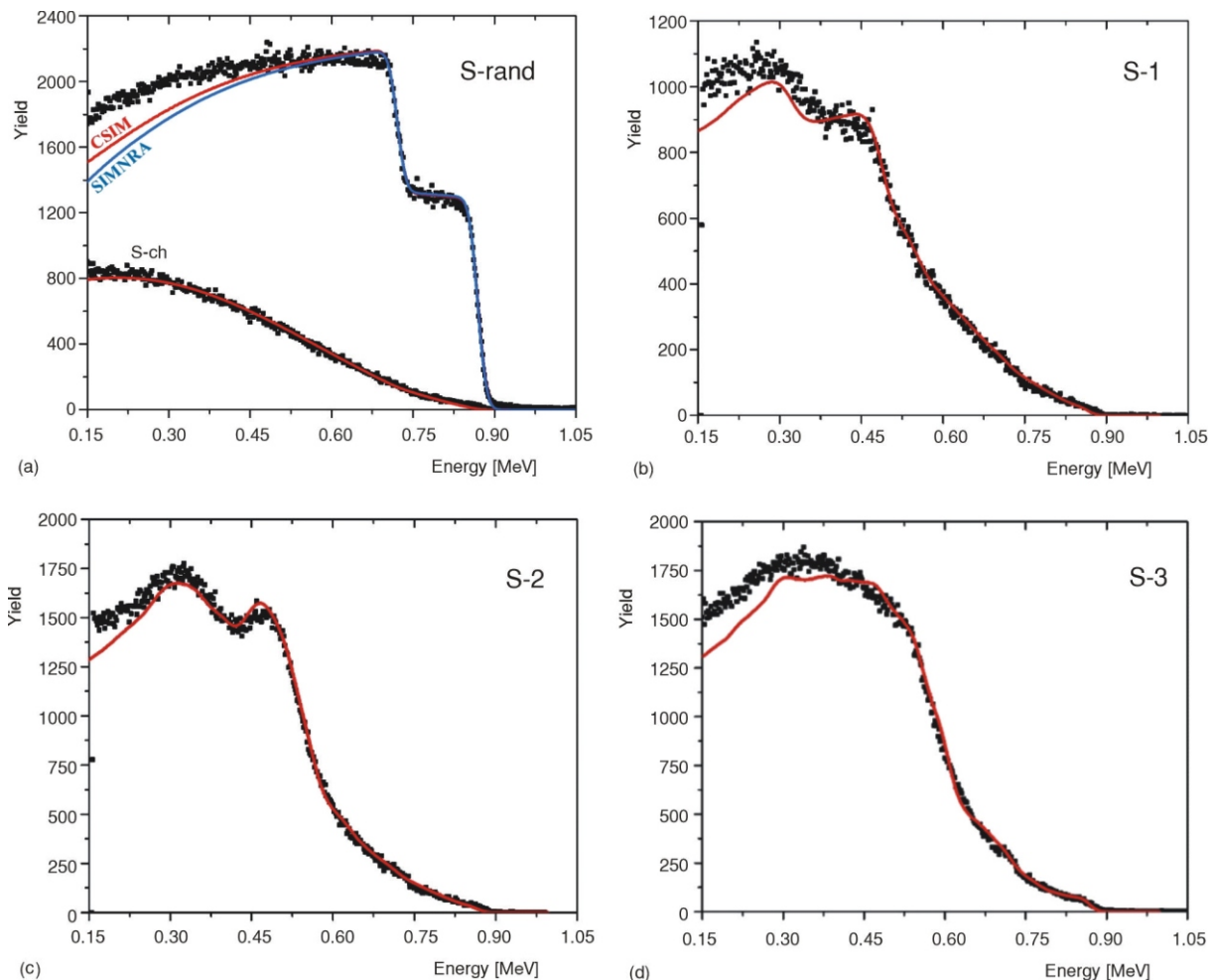


Figure 1. The BS/C spectra probed by 1 MeV protons of; (a) S-ch and S-rand, (b) S-1, (c) S-2, and (d) S-3 samples

code [25] (blue line) to compare results. The CSIM and SIMNRA generated spectra show very good agreement between the two codes. Both fitted spectra are exhibiting disagreement with experimental data at the spectrum's low energy range. The reason for this discordance can be found in the existence of multiple ions scattering events manifesting themselves in the spectrum's low energy range as an additional scattering, which neither computer code takes into account.

The BS/C spectrum of the non-implanted sample (S-ch) is also presented in fig. 1(a). Using the previously mentioned procedure of χ^2 minimization procedure, the channeling parameters are obtained. The channeling to random energy loss ratio (α) has the value of 0.84, while the dechanneling rate (k) and the dechanneling range (x_c) have the values of 0.32 m^{-1} and 3.54 m , respectively. The CSIM fitted S-ch spectrum exhibits a very good match with the experimental data. The BS/C spectra of implanted samples were also fitted by CSIM code using the aforementioned channeling parameter set (α , k , and x_c) and the results of the best-obtained fits are presented in fig. 1(b)-1(d). As it can be observed, fitted spectra in the spectrum's high energy range are showing an excel-

lent match with the experimental ones. The disagreement occurs at a low energy range, similarly to the previous case, due to the existence of the multiple scattering events. The BS spectrum of the non-implanted sample (S-rand) can be used to simulate the BS/C spectrum for the fully amorphized crystal structure. Consequently, the greater the crystal damage the more the BS/C spectrum of implanted sample resembles the BS spectrum of a randomly oriented crystal.

Damage depth profiles obtained from BS/C spectra shown in fig. 1(b)-1(d) using the CSIM code are presented in fig. 2(a). Profiles show asymmetric shape with a steeper edge on the side of higher depths and with the maximum at $2.8 \text{ m} - 3.1 \text{ m}$ for the S-1 sample and $2.8 \text{ m} - 3.0 \text{ m}$ for S-2 and S-3 samples. For the comparison purpose, SRIM simulation of 4 MeV C ion implantation induced damage in SiC is given. The SRIM obtained damage depth distribution is presented in fig. 2(a) together with appropriate CSIM profiles. The maximum damage profile obtained by SRIM is at 2.69 m and the profile's edge on the side of higher depths is even steeper in comparison to CSIM obtained profiles. Henceforth, the crystal damage depth profile induced by

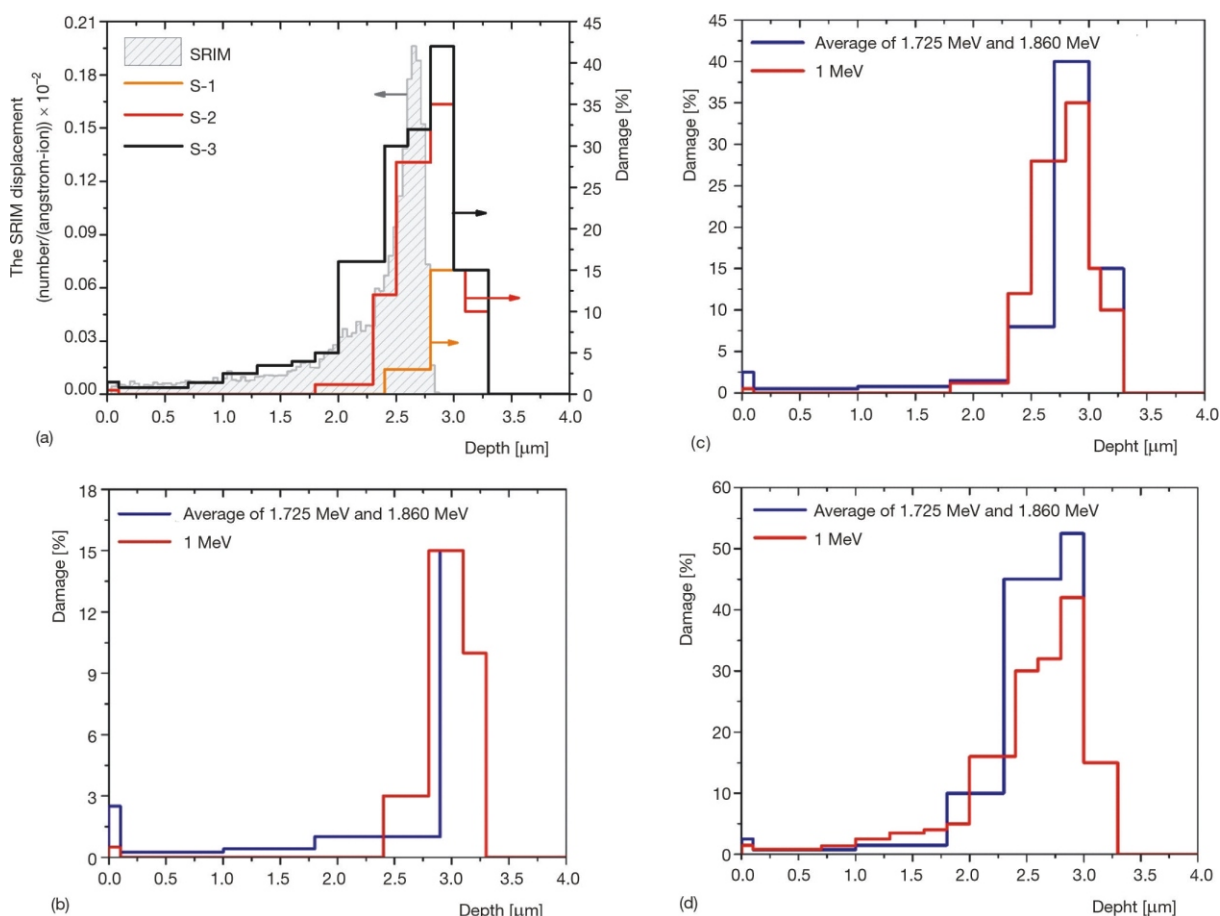


Figure 2. (a) Damage depth profiles obtained by fitting of BS/C spectra probed by 1.000 MeV protons of S-1, S-2, and S-3 samples by CSIM computer code; the CSIM profiles are compared with the damage profile obtained by SRIM simulation for 4 MeV C ion implantation in SiC; CSIM profiles of BS/C spectra probed by 1 MeV protons are compared with the one probed by 1.725 MeV and 1.860 MeV protons (their average profiles) [3] for (b) S-1, (c) S-2, and (d) S-3 samples

channeling implantation of 4 MeV C ions in 6H-SiC is shifted toward higher depths (0.3 μm) and is wider by about 0.8 μm in comparison to the damage profile induced by implantation in random.

The averaged CSIM 6H-SiC damage depth profiles probed by 1.725 MeV and 1.860 MeV protons are also shown in fig. 2(b)-2(d). These damage profiles were cross-checked by both R and SEM analysis, independently, showing very good agreement. The difference between averaged profiles probed by 1.725 MeV and 1.86 MeV protons and those probed by 1 MeV protons is reflected in the change of the damage intensity distribution. This difference increases with the increase of implanted fluence. However, the depth of maximum damage and damaged depth zone positions stay the same. The reason for this discrepancy between them can be found in the existence of strong resonant peaks in the 1.725 MeV and 1.860 MeV BS/C spectra originating from $^{12}\text{C}(p,p_0)^{12}\text{C}$ and $^{28}\text{Si}(p,p_0)^{28}\text{Si}$ nuclear reactions at 1.731 MeV and 1.667 MeV, respectively. The appearance of these prominent resonant peaks in the 1.725 MeV and 1.860 MeV proton BS/C spectra, has a role of a unique energy marker during the CSIM fitting procedure. The existence of the prominent minima and maxima in the BS spectrum limits the number of possible sets of channeling parameter values (α , k , x_c) for which the minimization procedure can converge to the unique solution. Therefore, CSIM profiles obtained from 1.725 MeV and 1.860 MeV proton BS/C spectra have higher accuracy. On the other hand, the existence of the prominent resonance peak is not suitable for the iterative procedure, because it needs a relative plateau in the random BS spectrum, which is used as a base for differentiation, to minimize the relative error. So, for the sake of comparison with the iterative procedure, we will use CSIM profiles obtained by 1 MeV BS/C spectra.

It was shown that the difference between the maximum of the damage profile for random and channeling implantation direction was about 0.3 μm , that is, about 10%. The reason for this relatively small difference between channeling and a random case could be found in the size of the (0001) 6H-SiC axial channel. The channel size is taken to be a geometric figure formed by the atoms of the wall of the crystal channel (channel nodes). According to the literature data for 6H-SiC(0001) and Si(110) axial channel dimensions [26], the Si(110) channel is about 7.5 times larger than the 6H-SiC(0001) one. Additionally, Kopsalis *et al.* [27] have shown that in the case of 5 MeV O^{2+} channeling implantation in Si(110), the difference between random and channeling implantation damage depth profile maximum is about 1 μm or about 20% of the position of its maximum. Therefore, by comparison, it is a justified appearance of a smaller difference of 10% in the case of the 6H-SiC(0001) channel in comparison to random orientation.

The main drawback of the iterative procedure for the determination of crystal damage depth profiles out-

side of the surface region (usually less than 1 μm in depth) is the difference between energy losses for channeled and non-channeled ions. However, in the case of 6H-SiC (0001) implantation, because of the small difference between random and channeling ion ranges, it was proposed that an iterative procedure can be applied for depths greater than 1 μm . The iterative procedure that was used in this paper is described in the study of Zhang *et al.* [28]. In principle, the iterative procedure is based on the separation of dechanneling contribution to the experimental spectrum yield from the one caused by crystal damage. For each iterative procedure calculation set, the BS/C spectrum of the implanted sample, BS, and BS/C spectra of a non-implanted sample of the same crystal are needed, fig. 3(a), for S-3 sample. Before the calculation of dechanneled contribution to the spectrum yield (R) can be done, yields of BS/C spectra of implanted and non-implanted samples need to be normalized to the yield of BS spectrum of the non-implanted, pristine, spectrum (N and V , respectively). Using the iterative procedure, the value of R is then obtained by [28]

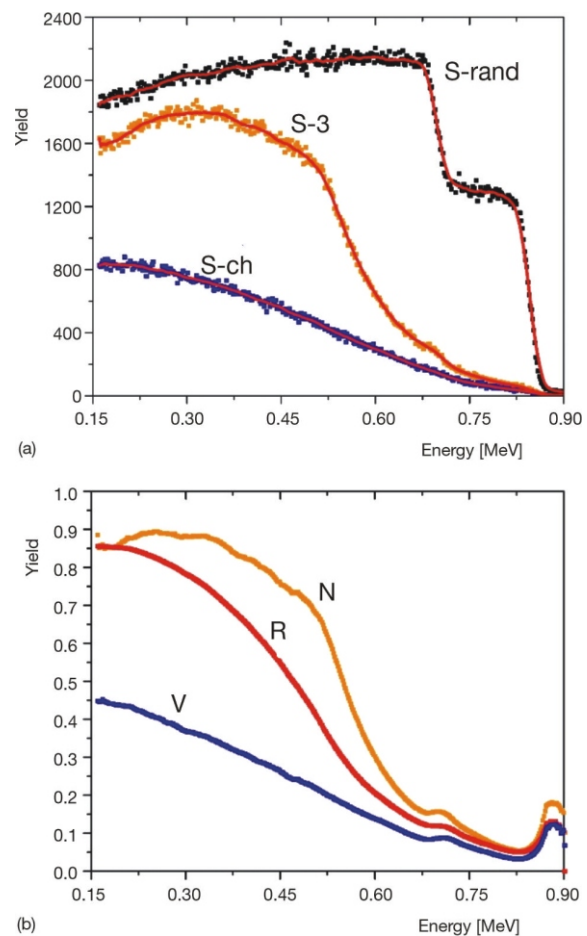


Figure 3. (a) BS/C spectra of S-ch, S-rand, and S-3 samples. Smoothed curves (red line) for these samples are also shown, (b) Normalized yield of S-ch (V) and S-3 samples (N) by S-rand yield and resulting backscattered dechanneling component (R)

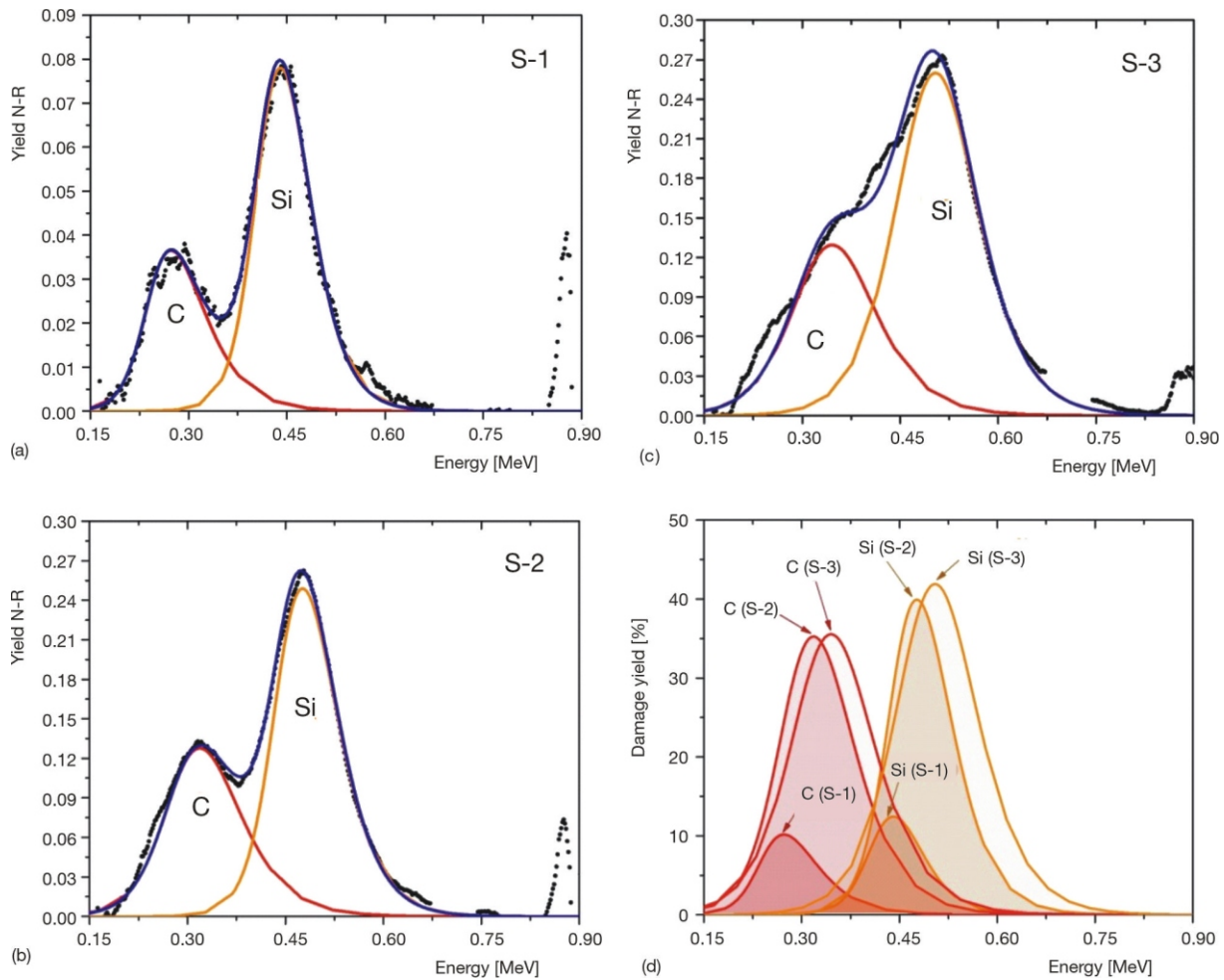


Figure 4. Damage yield curves fitted with two asymmetric bands which represent C and Si contributions for (a) S-1, (b) S-2, (c) S-3 samples, and (d) summarized result of contribution separation from (a)-(c) with applied damage yield normalization procedure

$$[1 - V(i)] \exp \left[-\sigma_{pp} \sum_{i=1}^n \frac{N(i-1) R(i-1)}{1 - R(i-1)} \right] = V(i) \quad (1)$$

where σ_{pp} is the parameter associated with the dechanneling cross-section along a particular crystal channel and i channel number/energy. Its value can be estimated in a spectrum region when the R curve overlaps with the N curve, right after the crystal damage spectrum region fig. 3(b). The spectrum yield component originating from the ion backscattering on crystal damage/impurities can be obtained by subtracting the values R from N for the same energy. The first *step* of SiC BS spectrum yield originates only from the Si atoms, however, the second *step* originates from both Si and C atoms. Therefore, a corresponding correction to the damage yield must be done [28]. The damage yield from the first *step* in the BS/C spectrum was normalized taking into account the second *step* height. However, the second, C, step causes prominent oscillations in the iterative procedure, which is differential in its

nature. To reduce these oscillations of two consequential iteration steps, experimental spectra were smoothed before the iterative procedure using an adjacent-averaging method with 20 points per step.

The results of the iterative procedure are presented in fig. 4(a)-4(c). Damage yield in the region of the first *step* is practically negligible. A majority of the damage yield is placed in the region of the second spectra *step*. Due to different atomic masses of Si and C, the damage yield for C and Si atoms (crystal sublattice) is shifted in spectra. In the case of S-1 and S-2 samples figs. 4(a) and 4(b) the contribution belonging to C and Si sublattices is distinctively separated. The maximum damage yield for the C sublattice of the S-1 sample is at 0.27 MeV, while for the S-2 sample is at 0.32 MeV. For Si sublattice, the maximum damage distribution is at 0.44 MeV for the S-1 sample and at 0.47 MeV for the S-2 sample. However, in the case of the S-3 sample fig. 4(c), it is not that straightforward, since the highest implanted fluence contributed to the most pronounced crystal damage resulting in the overlap between damage distributions of both sublattices. To extract contribution for each atom for

all samples, a fitting procedure with two bands approximated with an asymmetrical function has been performed

$$I = I_0 + B \left[1 - \exp\left(-\frac{x - x_c}{k_2}\right) \right] + \left[1 - \exp\left(-\frac{x - x_c}{k_3}\right) \right] \quad (2)$$

where I represent yield, I_0 baseline value, B amplitude, x energy/depth values, x_c peak center, and k_{1-3} values of specific profile widths. The usage of asymmetric function for extraction of damage yield is justified by the asymmetrical shape of the damage profile, which is usual for ion implantation-induced crystal damage, see fig. 2(a), SRIM data simulation. The discontinuities in the 0.67 MeV-0.74 MeV energy region of N-R damage distributions relate to the abrupt increase of spectra yield from C atom backscattered. To avoid the introduction of uncertainties in further crystal damage analysis, the yield from this region was omitted.

Contributions from C and Si crystal sublattice to the damage have different heights because of the different values of their cross sections. To normalize the contribution for each sublattice, elemental BS spectra obtained by SIMNRA spectrum from fig. 1(a) was used. Partial spectra yield contributions for C and Si sublattices are presented in fig. 5. Normalization of the C and Si sublattice yield was done by using the characteristic value of C and Si contribution from fig. 5. The yield from the Si spectrum *step* was normalized to C spectrum *step* yield to make yield separation originating from different elements. The summarized results after yield normalization are presented in fig. 4(d). It was expected that after damage yield normalization, C

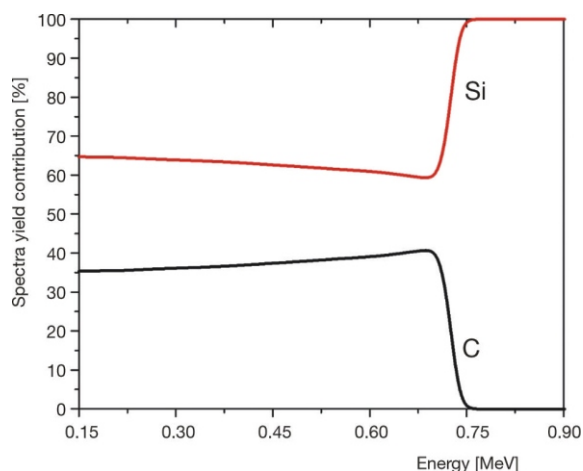


Figure 5. Degree of the spectra yield contribution for C and Si sublattice obtained from elemental BS spectra by SIMNRA simulation of the spectrum from fig. 1(a)

and Si sublattices would have had similar damage depth distributions. Instead, damage profile intensities manifested in C and Si sublattices exhibit a difference of 12-17 % depending on the sample. These differences can be ascribed to the multiple scattering processes which manifest themselves at low spectrum energies where consequently C sublattice spectra yield is more dominant. Therefore, Si sublattice damage profiles will be used for comparison with CSIM obtained ones. With the increase of implanted fluence, one can observe the increase of crystal damage and its spreading towards higher spectrum energies. This is indicative of the so-called dynamic effect during the channeling ion implantation. Namely, with the increase of the implanted fluence, the crystal channels deteriorate causing more pronounced energy loss that subsequently channeled ions experience, leading to shorter achieved ranges and crystal damage shift towards the crystal surface. These results show good agreement with previous studies [3, 29].

Previously, the separated damage profiles vs. energy of backscattered protons for each target atom were presented. However, to obtain a crystal damage depth profile, crystal damage vs. crystal depth, the energy to crystal depth conversion has been done. This energy to crystal depth conversion is based on stopping values for protons in the SiC taken from SRIM. The conversion could be done by having the same energy loss rate for channeled and non-channeled ions, as is the default assumption for the iterative procedure and its main drawback for higher crystal depths, or with the correction factor in the way of channeling to random energy loss ratio (α), which takes into account the different energy loss rates for channeled and non-channeled ions. In the case of energy loss correction, the fact that at the same crystal depth there would be different energy at which protons would be undergoing the scattering event than in the case without, leads to different values of scattering cross-sections. Therefore, alongside the shift in the crystal depths of damage profiles obtained with and without energy loss correction, there would be a shift in their height as well.

Damage profiles obtained by an iterative procedure, using Si sublattice profile, after energy-depth conversion are presented in fig. 6(a)-6(c) together with corresponding CSIM profiles of 1 MeV proton BS/C spectra. For each investigated sample, profiles are shown without ($\alpha = 1$) and with ($\alpha < 1$) channeling correction factor. In the case of profiles with included corrections, the value of α is taken to be 0.84 as was obtained by the χ^2 minimization procedure using CSIM. Differences between profiles with and without energy loss correction concerning the position of profile maxima are about 0.2 μm , *i. e.*, about 7 %, while the change to the profile heights due to correction is minimal, less than 1 %. The CSIM damage profiles compared with the profiles obtained via iterative procedure with energy loss correction ($\alpha = 0.84$) show ex-

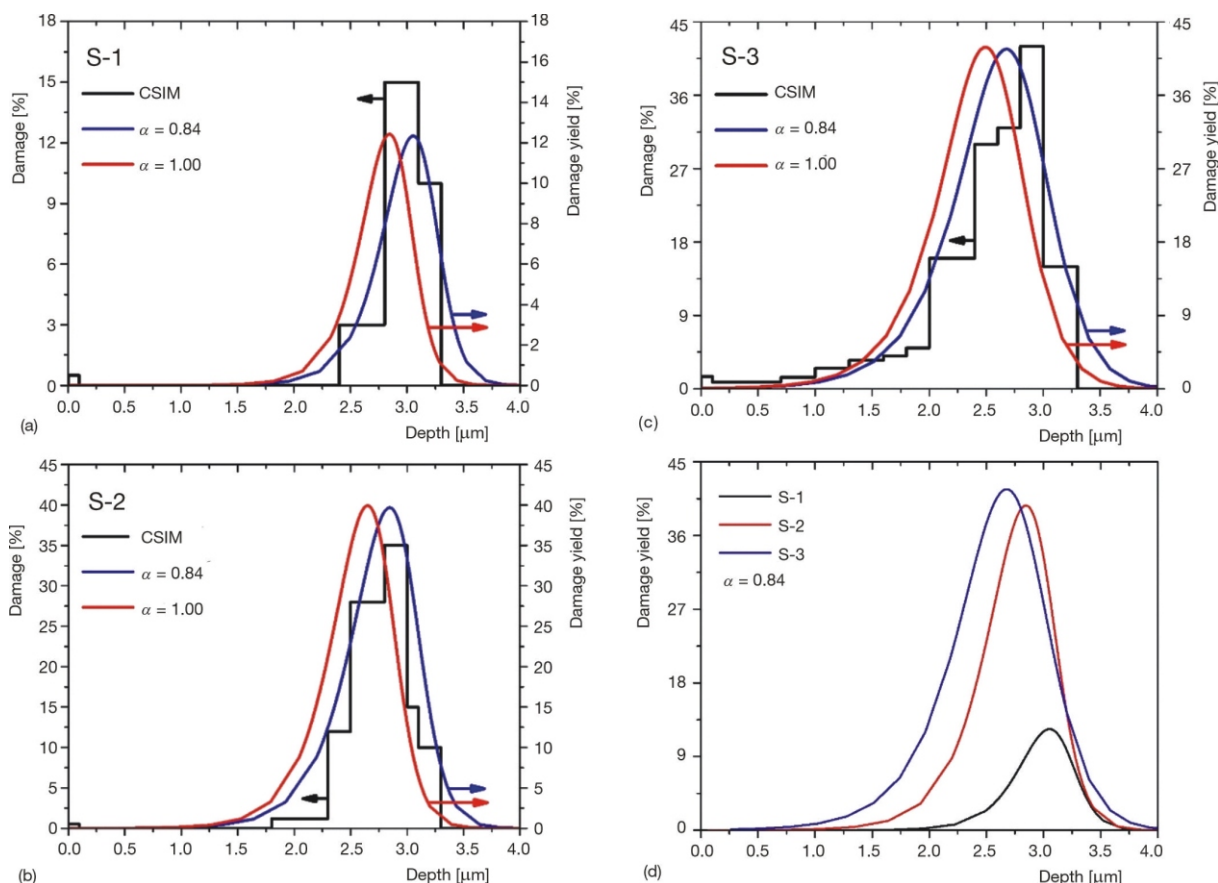


Figure 6. Comparison of damage yield depth profiles obtained by the iterative procedure for $\alpha = 1$ and $\alpha = 0.84$ and CSIM damage depth profiles for samples; (a) S-1, (b) S-2, (c) S-3, and (d) comparative result for all damage yield depth profiles obtained by an iterative procedure

cellent agreements, both for the maxima position and the total crystal damage, the difference in the degree of crystal damage is less than 5%. This is a confirmation of the successful usage of the iterative procedure in this specific case of BS/C spectra analysis. The overview of all damage profiles obtained by an iterative procedure for $\alpha = 0.84$ is shown in fig. 6(d). It can be observed that the trend of increase of the crystal damage with fluence follows the one obtained by the CSIM code as shown in fig. 2(a).

CONCLUSIONS

The BS/C spectra recorded with 1 MeV protons of 6H-SiC crystal implanted in (0001) axial direction by 4 MeV C^{3+} ions are analyzed by CSIM computer code and by an iterative procedure. Depth profiles obtained by CSIM code show very good agreement with previously extracted damage profiles from BS/C spectra probed by 1.725 MeV and 1.860 MeV protons. Due to the small difference between damage profiles induced by implantation in channeling and random crystal direction, the iterative procedure for analysis of

BS/C spectra has been proposed for greater crystal depths than those for which this analytical method was commonly used. Crystal damage depth profiles obtained by it show good agreement with CSIM results. These are further improved with the introduction of the energy loss correction factor in energy to crystal depth conversion (α , channeling to random energy loss ratio obtained by χ^2 minimization procedure). In this case, the agreement between the iterative procedure and CSIM profiles is excellent, both regarding the profile maximum position and profile height. We have shown successful usage of the iterative procedure in determining the crystal damage profiles for greater depths than 1 μm in the case when channeling and random implantation ranges do not differ too much (in this case, the difference was about 10%).

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AUTHORS' CONTRIBUTIONS

The concept for the paper originated with M. V. Erich, M. P. Gloginjić, and S. M. Petrović. The supervision was provided by S. M. Petrović, K. Katovský, and B. Vrban. Experimental measurements were done by S. M. Petrović. The RBS and EBS spectrum simulation computer code was written by M. V. Erich and M. P. Gloginjić. M. P. Gloginjić, Ž. V. Mravik, J. Lüleý, J. Burian, and V. Filová performed numerical analysis. Š. Čerba and O. Štastný reviewed and assessed all analytical results. M. P. Gloginjić has written the initial draft of the manuscript. All authors reviewed and discussed the manuscript.

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**Марко П. ГЛОГИЊИЋ, Марко В. ЕРИЋ, Жељко В. МРАВИК,
Бранислав ВРБАН, Штефан ЧЕРБА, Јакуб ЛУЛЕИ, Вендула ФИЛОВА,
Карел КАТОВСКИ, Ондреј ШТАСТНИ, Јиржи БУРИЈАН, Срђан М. ПЕТРОВИЋ**

**УПОРЕДНА СТУДИЈА ОШТЕЋЕЊА 6H-SiC ПРОУЗРОКОВАНА
ИМПЛАНТАЦИЈОМ MeV-СКИХ ЈОНА ПРИ ОРИЈЕНТАЦИЈИ
КАНАЛИСАЊА КОРИШЋЕЊЕМ ИТЕРАТИВНОГ ПОСТУПКА И
ФЕНОМЕНОЛОШКОГ CSIM ПРОГРАМСКОГ КОДА**

Због својих јединствених карактеристика, као што су екстремна тврдоћа и отпорност на зрачење, силицијум карбид (SiC) користи се као важан конструкциони материјал у окружењима изложеним екстремним условима, попут оних у нуклеарним реакторима. Као такав, стално је изложен енергетским честицама (на пример неутронима) и последично подвргнут постепеној деградацији кристалне решетке. У овом чланку, оштећење кристала 6H-SiC симулирано је имплантацијом 4 MeV C³⁺ јона у (0001) аксијалном правцу монокристала 6H-SiC, флуенсима од $1.359 \cdot 10^{15} \text{ cm}^{-2}$, $6.740 \cdot 10^{15} \text{ cm}^{-2}$, и $2.02 \cdot 10^{16} \text{ cm}^{-2}$. Имплантирани узорци су накнадно анализирани помоћу Ратерфордове и еластичне спектроскопије повратног расејања при оријентацији каналасања (RBS/C & EBS/C) коришћењем протона енергије 1 MeV. Добијени спектри су анализирани феноменолошким програмским кодом CSIM (Channeling SIMulation) како би се добили квантитативни дубински профили оштећења кристала. Разлика између позиција максимума профила оштећења добијених помоћу CSIM кода и оне симулиране помоћу SRIM-a (Stopping and Range of Ions in Matter), програмског кода базираног на Монте Карло методи који је фокусиран на симулацију имплантације јона само у насумичном правцу кристала, износи око 10 %. Стога, због малих помераја дубине профила, предложено је коришћење итеративне процедуре за израчунавање дубинских профила оштећења кристала. Показало се да се профили добијени итеративним поступком веома добро слажу са профилима добијеним CSIM кодом. Поред тога, са увођењем односа енергијских губитака за каналасање и случајни правац имплантације при конверзији енергетске скале профила у скалу дубина, слагање са CSIM профилима постаје одлично.

Кључне речи: Силицијум карбид, рачунарска симулација, итеративни поступак, RBS/C и EBS/C спектрометрија
