

# Calibration of Aluminum Ion Implantation Monte-Carlo Model for TCAD Simulations in 4H-SiC

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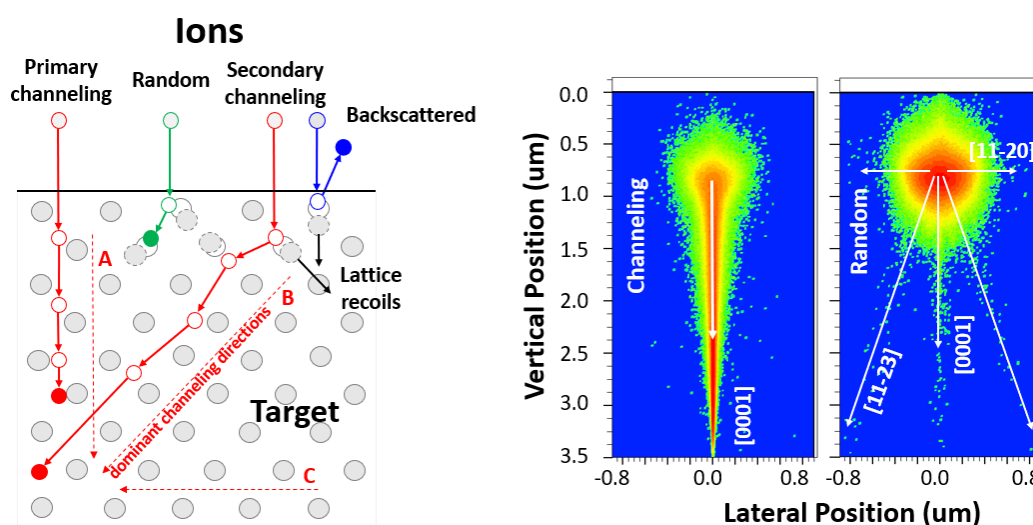
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## Introduction

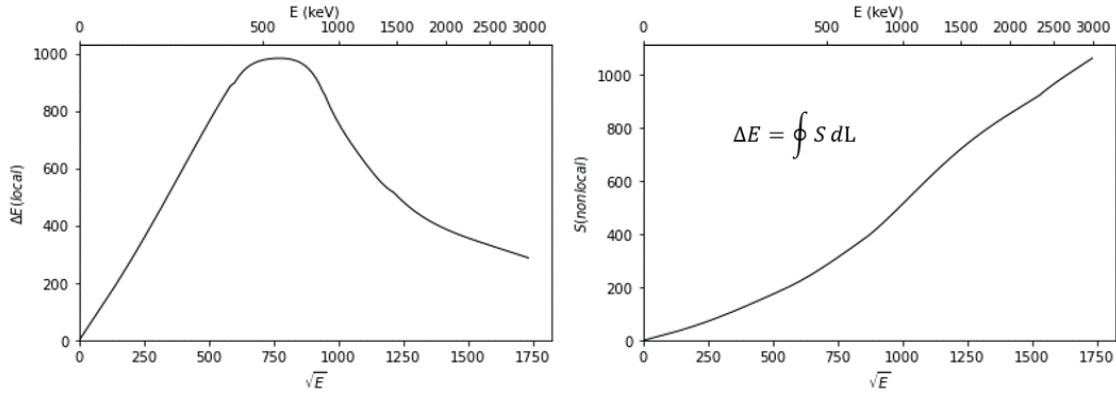
Ion implantation, as a way of doping the 4H-SiC crystal, is one of the key components of modern power device fabrication. Aluminum is used to form p-type wells for the body of n-MOSFETs and low resistance p-type contacts using heavy doping. Therefore, the ion implantation process needs to be controlled over a wide range of process conditions including implant energies and doses. The fact that Al in 4H-SiC exhibits very low diffusion puts additional burden on the accuracy and predictability of any ion implantation engineering. In device design, these requirements can be addressed by applying computer simulations to predict doping profiles ahead of the actual implant step performed in a manufacturing facility. The accepted way to predict doping profiles is based on the binary-collision approximation (BCA), numerically implemented as a statistical Monte-Carlo (MC) method [1]-[3]. Nowadays, one can refer to simulation packages available from commercial vendors [4] for studying ion implantation using BCA-MC algorithms. However, while the physical accuracy of BCA models implemented in these packages has shown to be quite remarkable, predictable simulations for a complex material system as 4H-SiC requires calibration from data including secondary ion mass spectrometry (SIMS) and scanning electron microscopy (SEM).

## Monte-Carlo Implant Simulations using BCA



**Fig. 1.** Left: Possible scenarios for ion scattering in a crystalline material with distinct channels. Right: 2D probability distributions (point responses) for implanted Aluminum ions in 4H-SiC. [0001] channeling vs. random distribution.

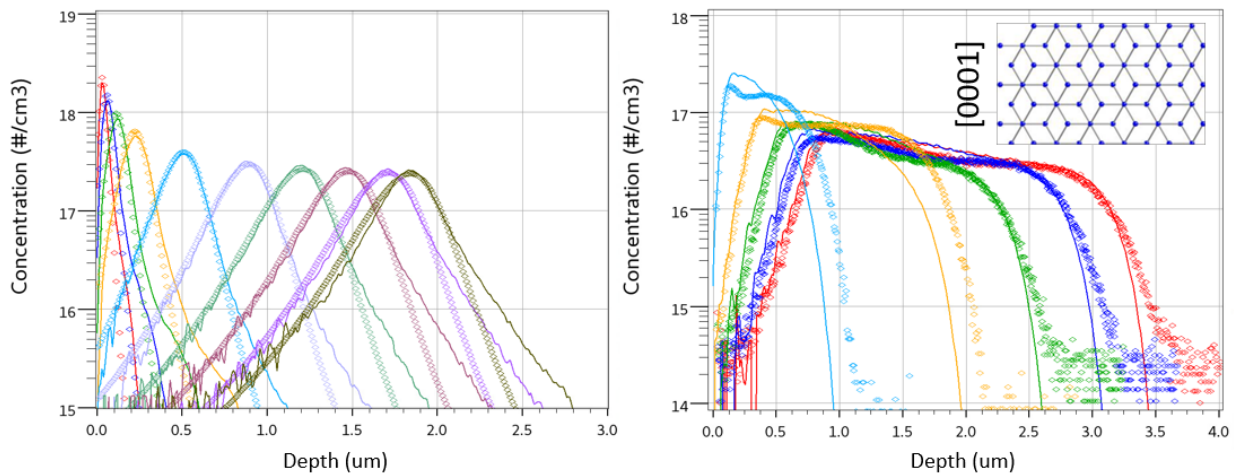
A complete calibration of the BCA method has to address both depth profiles and the lateral distribution for junction formation of implanted species [3]. In addition to random scattering, the channeling (Fig. 1, left) is of key importance for a correct representation of doping profiles in all space dimensions. In this work, we demonstrate the use of a wide range of SIMS data for different implant conditions spanning energy ranges of 50 keV to 2.8 MeV outside the main channels (random profiles) [5], as well as a limited dataset for implantation into the main channeling directions [0001] and [11-23] 4H-SiC [6]. We discuss the electronic stopping for random profiles with little to no channeling components (Fig. 1 right). The addition of data for the main channels is of importance



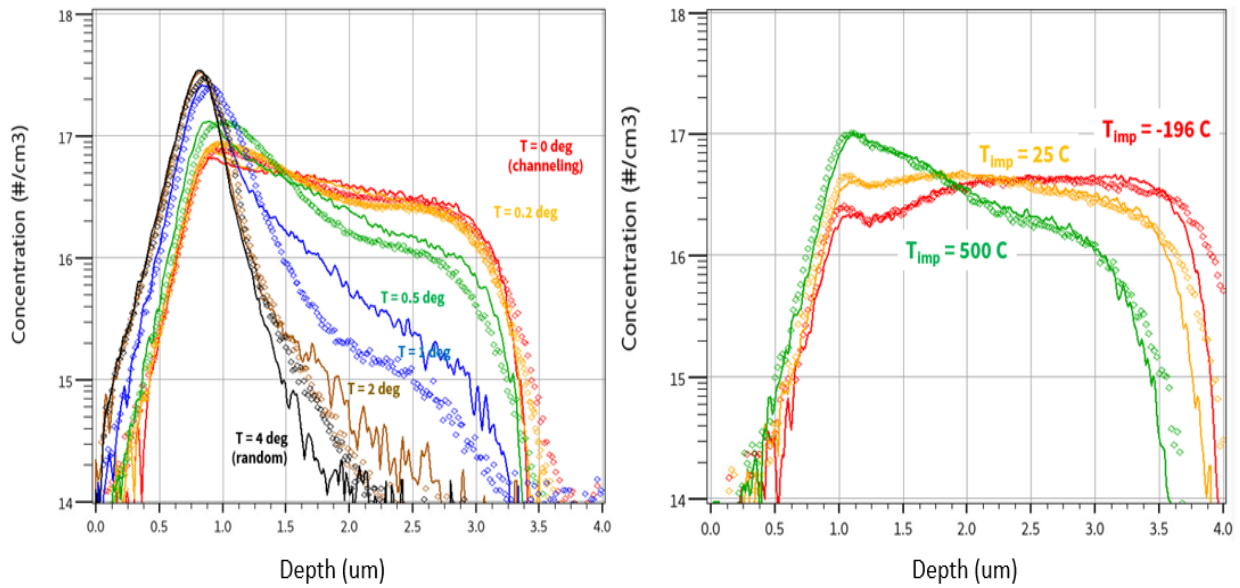
**Fig. 2.** Left: Energy loss due to local electronic stopping as a function of the implant energy. The energy loss  $\Delta E$  is given in eV. Right: Non-local stopping power as a function of the square root of the implant energy. The energy loss in eV is the path integral of the stopping power along the ion trajectory.

since accurate predictions of implant depth and lateral straggle depend on the calibration of ion stopping in the channeling directions (Fig. 1, middle). It is known that when channeling occurs, ion stopping is less strong, resulting in deeper doping profiles. We use the local electronic stopping due to kinetic momentum transfer at low energies and the non-local stopping at high energies as the main physical mechanisms for calibration (Fig. 2). Implant temperature dependence of the implant profiles is considered through a standard damage accumulation model with a dynamic amorphization threshold. The calibration presented will cover low temperature (-196 °C) and high temperature (500 °C).

## Results of the BCA Calibration

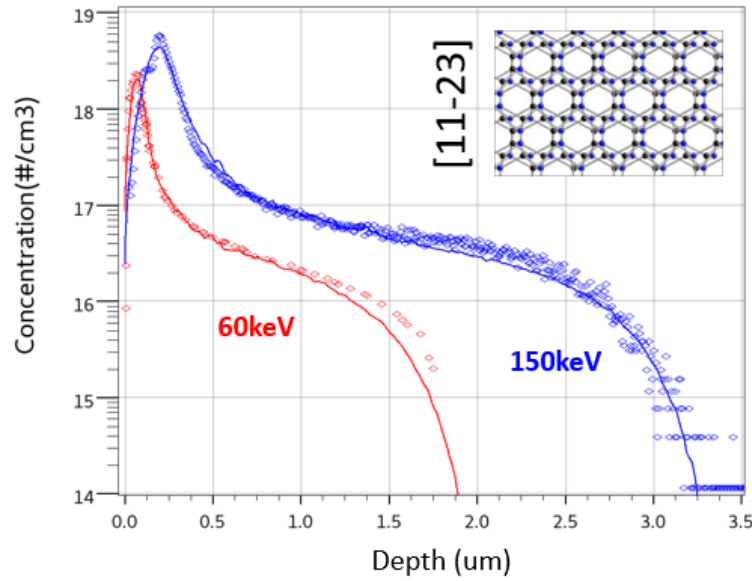


**Fig. 1.** Left: Random doping distributions for Al from 50 keV to 2.8 MeV,  $1e13\text{cm}^{-2}$  dose from [5] (markers) overlaid with the curves from the calibrated BCA simulations. Right: [0001] channeling doping distribution for Al from 100 keV to 900 keV [6]. SIMS data (markers) overlaid with BCA simulations. The inset shows the atomic lattice projected along the [0001] crystalline direction in 4H-SiC.



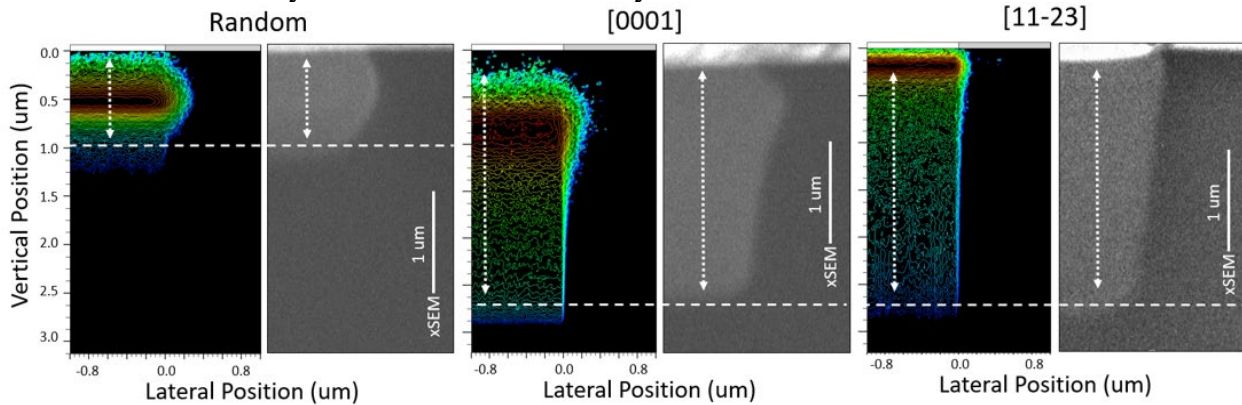
**Fig. 4.** Left: Doping distributions for Al, 900 keV transitioning from a strong channeling regime to a random regime by changing the tilt angle w/r to the [0001] crystal orientation [6]. Right: Implant temperature dependence of [0001] channeled profiles for -196 °C, 25 °C, and 500 °C. Overlay with SIMS data for 1.2 MeV,  $1 \times 10^{13} \text{ cm}^{-2}$  dose.

Fig. 3 (left) shows implant profiles in the non-channeling, random crystal from [5] overlaid with the profiles from the calibrated model. This is used to establish the first order energy dependence of electronic stopping for Aluminum in 4H-SiC as shown in Fig. 2. The BCA model treats the electronic stopping in the [1100] and the [11-23] channel as a direction-dependent modification of the strength of the random electronic stopping relation. The relative strengths of electronic stopping (both local and non-local) in the channels vs random direction will be established based on SIMS data for these channel directions (Figs. 3(right), 4 and 5). The results shown in Fig. 4 (left), for instance, demonstrate the BCA model response as compared to SIMS profiles for several tilt angles between the random direction and the [0001] channel direction to demonstrate the effect of de-channeling. The implant temperature dependence of the impurity profiles in the [0001] channel is shown in Fig. 4 (right). The impurity profiles from stopping in the [11-23] channel, which is oriented 17 degrees from the [0001] direction, is given in Fig. 5. The non-local electronic stopping in the [11-23] channel has been adjusted to match the tail distributions in the simulations to the SIMS profiles.



**Fig. 5.** [11-23] channeling doping distribution for Al for two different energies, 60 keV and 150 keV,  $1 \times 10^{14} \text{cm}^{-2}$  dose. The inset shows the atomic lattice projected along the [11-23] crystalline direction in 4H-SiC [4].

Finally, we compare the complete 2D profile shapes, including the lateral component, from SEM for a random, a [0001] channelled, and a [11-23] channelled implant with the results from the calibrated BCA model for Aluminum (Fig. 6). The energies for the channeling measurements and simulations are chosen such that the same profile depth for the [0001] and the [11-23] direction is achieved. The impurity profile depth and lateral distribution are very well reproduced by the Monte-Carlo simulations. This clearly demonstrates the accuracy of the calibrated BCA model.



**Fig. 6.** 2D profiles for Aluminum implantation at an ideal mask edge. (a) Random distribution, 500 keV; (b) channeling in [0001], 700 keV; (c) channeling in [11-23], 150 keV. All doses are  $1 \times 10^{14} \text{cm}^{-2}$ . The corresponding SEM cross-sections are displayed to the right of each TCAD representation.

## Summary and Outlook

A calibrated framework for the simulation of ion implantation of Aluminum in 4H-SiC power devices is presented. Based on a commercially available implantation simulation software [4], comprehensive calibration of the BCA-MC method was performed for a broad range of implant conditions such as energies, doses and temperatures. Electronic stopping, both local and non-local in nature, alongside damage and amorphization have been shown to be the main physical mechanisms to be considered for predictive modeling of impurity profiles in 4H-SiC. The revised model shows a very good agreement with measured SIMS profiles. In addition, it has been shown that the lateral profile accuracy requires calibrations of the main channels in the 4H-SiC crystal. We included SIMS

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data for the [0001] and the [11-23] channel. The latter is in particularly important for accurate simulations of lateral profiles since it is directed 17 degrees off the main wafer direction which is aligned with the <0001> crystal orientation. Suggested future work should include data from the [11-20] channel which is oriented perpendicular to the <0001> wafer orientation and therefore plays an important role in the understanding of lateral scattering in 4H-SiC.

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