Supplementary material for

Microscopic origin of the acceptor removal in neutron-irradiated Si detectors - An atomistic simulation study

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I. Modeling of intrinsic defects and defect-dopant interactions

In our object kinetic Monte Carlo (kMC) model, the mono-vacancy (V), the mono-interstitial (I), the di-interstitial (I_2), the tri-interstitial (I_3) and the boron-interstitial (B_i) are considered as mobile defects. The migration energies of these defects are summarized in Table S1 and are taken from [1, 2].

C and O impurities are modeled as traps for intrinsic defects and dopants by the formation of C_i ($C + I \leftrightarrow C_i$), VO ($V + O \leftrightarrow VO$) and B_iO ($B_i + O \leftrightarrow B_iO$) defects. The binding energies of these defects are included in Table S2.

The second-neighbor distance of the Si lattice (0.384 nm) is used as the jump distance for mobile species, and as capture radius for any interaction between intrinsic defects, dopants and impurities [3]. When both B and C atoms lie within the interacting radius of a Si interstitial, priority is given to the I-B reaction to reflect the higher capture radius of interstitials at B than at C [4].

When defects of the same type interact they form agglomerates (clusters) of Si self-interstitials ($I_{1,2,3} + I_n \leftrightarrow I_{n+1,2,3}$) or vacancies ($V + V_n \leftrightarrow V_{n+1}$) whose evolution is controlled by the formation energies of the different cluster sizes. In our model, we consider only the energetics of the most stable cluster configuration of a particular size. However, several configurations of a given cluster size may coexist [5, 6] since there are energy barriers for configurational transitions that hinder the evolution to the most stable ones [7].

The formation energies of small vacancy clusters used in our model are reported in Table S3 and were taken from Ref. [8]. For small Si self-interstitial clusters, the formation

energies were extracted from Ref. [9] and are summarized in Table S4. Other sets of clusters energetics have been proposed in literature (for instance, Staab *et al.* [10], Hasting *et al.* [11] and Lee *et al.* [12] for vacancy clusters, or Colombo *et al.* [13], Chichkine *et al.* [14] and Martín-Bragado *et al.* [15] for Si self-interstitial clusters), which result in different cluster kinetics at elevated temperatures [1]. However, at the temperatures used in this work (RT or 60 ºC) once clusters are formed they hardly dissolve and, therefore, our results are insensitive to the specific energetics used.

In our model, the interaction of mobile Si self-interstitials (I_{mob}) and B_i with B atoms results in the formation of B-I clusters, which may also grow by incorporating additional Si self-interstitials or B atoms. The energetics of small B-I clusters are reported in Table S5 and are taken from [1].

Table S1. Migration energies (E_m) of mobile point defects.

	V	I	I_2	I_3	B_i
E_m (eV)	0.43	0.9	0.5	0.6	0.7

Table S2. Binding energies (E_b) of dopant and impurity point defects.

	B_i	B_iO	VO	C_i
E_b (eV)	1.0	0.7	2.3	1.5

Table S3. Formation energies (E_f) of small vacancy clusters (V_n) referred to the perfect lattice.

	V	V_2	V_3	V_4	V_5	V_6	V_7	V_8	V_9	V_{10}
E_f (eV)	3.65	5.7	7.9	10.4	11.9	12.9	15.4	16.0	16.9	18.0

Table S4. Formation energies (E_f) of small Si self-interstitial clusters (I_n) referred to the perfect lattice.

	I	I_2	I_3	I_4	I_5	I_6	I_7	I_8	I_9	I_{10}
E_f (eV)	3.8	6.1	7.9	9.2	10.7	12.3	13.9	14.8	16.5	17.9

Table S5. Formation energies (E_f) of small boron-interstitial clusters (B_nI_m) referred to the perfect lattice.

	B	B_i	BI_2	BI_3	B_2	B_2I	B_2I_2	B_2I_3	B_3	B_3I	B_3I_2	B_3I_3
E_f (eV)	0	2.8	5.2	7.0	0.9	2.1	4.4	6.8	1.7	0.8	2.0	3.5

II. Concentration of defect clusters in neutron-irradiated p-type Si

Our atomistic kMC simulations provide the concentration of all defects considered in the model that result from 1-MeV neutron irradiation in Si. Of particular significance for B deactivation are the concentration of mobile Si interstitials and defect clusters (reported in Fig. 5 in the manuscript). For the analysis of intrinsic defects that can contribute as deep acceptors, the concentration and size distribution of vacancy and Si self-interstitial clusters is relevant (shown in Fig. 6 in the manuscript).

Defect concentrations obtained in simulations as a function of neutron fluence are fitted to power equations using α and β as fitting parameters:

$$C_{Cl}[cm^{-3}] = \propto \cdot \emptyset_{eq}^{\beta}[cm^{-2}] \quad (1)$$

where C_{Cl} is the defect concentration and $\emptyset_{eq}$ the 1-MeV Non-Ionizing Energy Loss (NIEL) equivalent fluence. The parameter α is indicative of the generation rate of the defect and β is related to the linearity of the dependence with fluence. The values of α and β for the concentration of mobile Si self-interstitials, defect clusters, and different

sizes of vacancy and Si self-interstitial clusters resulting from simulations are compiled in Table S6.

α and β parameters corresponding to small vacancy and Si self-interstitial clusters are also plotted in Fig. S1 and compared to those associated to the experimental introduction rate ($g_c \sim 0.02$ cm^{-1}) of deep acceptors ($\alpha = 0.02$ cm^{-1}, $\beta = 1$). They can be used to compare the introduction rate of intrinsic defects obtained in our simulations with that of deep acceptors or specific defects characterized by DLTS, TSC and other experimental techniques.

Table S6. α and β parameters from the fitting to power equations of mobile Si interstitials (I_{mob}) and defect cluster concentrations of Fig. 5 and the concentration of the vacancy and Si self-interstitial clusters reported in Fig. 6 (Fig. 5 and 6 are included in the manuscript).

	I_{mob}	Clusters	V_2	V_3	V_4	V_5	V_6	V_7	I_4	I_5	I_6	I_7
α	8227	145	19.87	5.73	2.41	0.06	0.02	0.01	1.15	0.03	0.01	5×10^{-4}
β	0.77	0.88	0.91	0.94	0.97	1.01	1.04	1.07	0.98	1.07	1.07	1.14

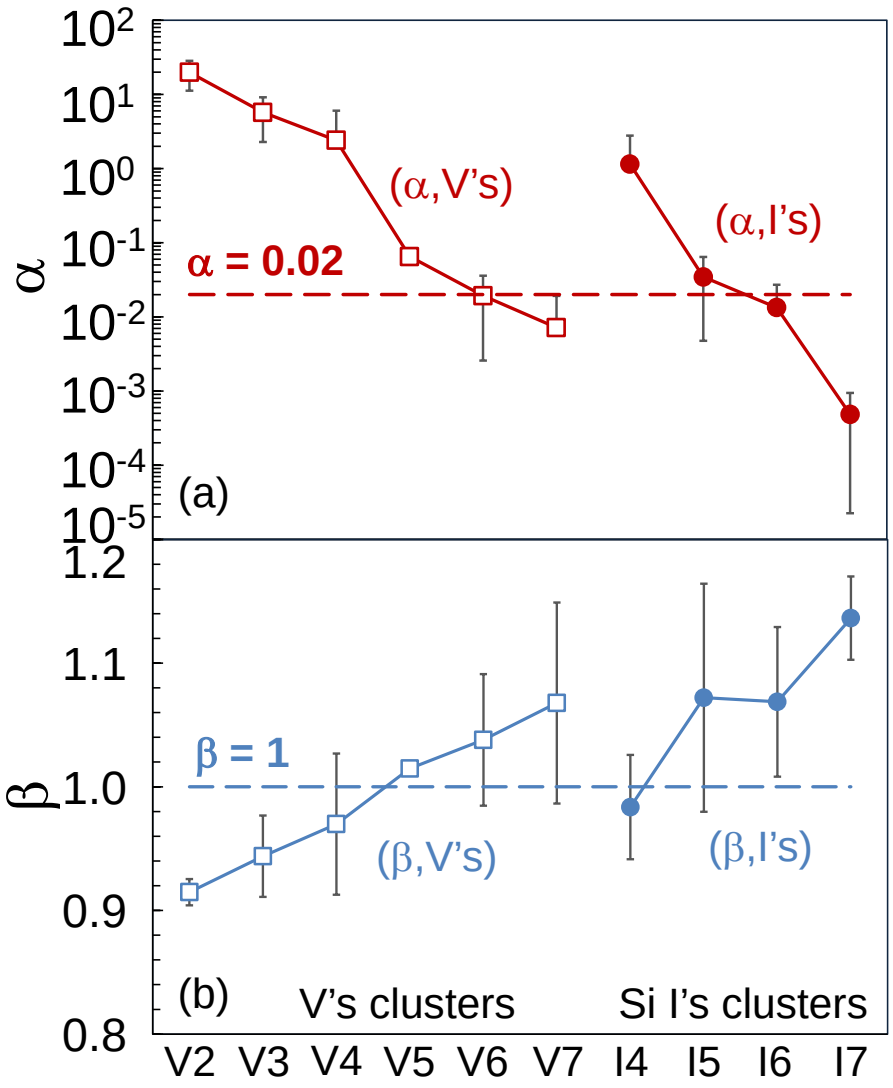

Figure S1. α (a) and β (b) parameters obtained from the fitting of cluster concentrations to power equations according to equation $C_{Cl}[cm^{-3}] = \propto \cdot \emptyset_{eq}^{\beta}[cm^{-2}]$. Vacancy and Si self-interstitial clusters are indicated as squares and circles, respectively. Data are averaged values from simulations with a $N_{eff,0}$ of 10^{13}, 10^{15}, 10^{17} B cm^{-3}, and error bars correspond to standard deviation. Dashed lines indicate α and β parameters associated to deep acceptors from the experimental g_c rate (α = 0.02 cm^{-1}, β = 1).

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