Supplementary Materials : Comparative study of collision cascades and resulting displacement damage in GaN, Si and Ge

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In this document, we regroup the data of the article for the 1 keV and 25 keV cascades, as well as the parameters used to construct the Tersoff/ZBL potentials. First, the box plots on the maximum penetration depth are exposed. Secondly, we present the box plots of the number of defects at the end of the collision cascades. Next, we show the evolution profiles of the number of defects as a function of the time. The visual representations of the defect clusters, the distributions of the number of clusters as a function of their size and the distributions of interstitial displacement distances are then shown. And finally, we discuss the coupling parameters of the Tersoff/ZBL potential used in this study. At 25 keV, data are derived from averaging results across 100 simulations for Ga and Ge PKAs, 85 simulations for Si PKAs and 82 simulation for N PKAs.

S.I Maximum penetration depth

Figures S1 and S2 show the maximum penetration depth distribution of PKAs at 1 keV and 25 keV for Ga and N PKAs in GaN, Si PKAs in Si and Ge PKAs in Ge.

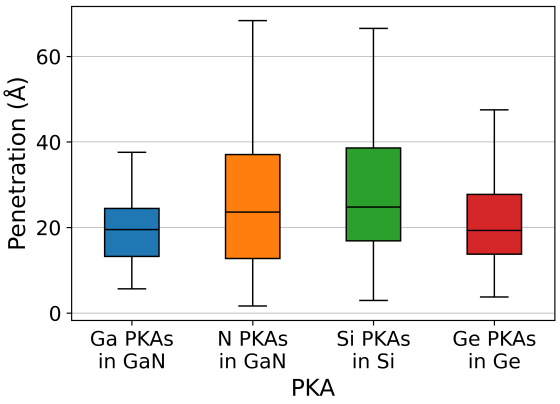

Fig. S1. Box plots of the maximum penetration depth of Ga PKAs in GaN (blue), N PKAs in GaN (orange) , Si PKAs in Si (green) and Ge PKAs in Ge (red) for 10 keV collision cascades. From lowest to highest, the horizontal lines of a box plot represents the minimum value of the set, the first quartile value, the median, the third quartile, and the maximum value of the set.

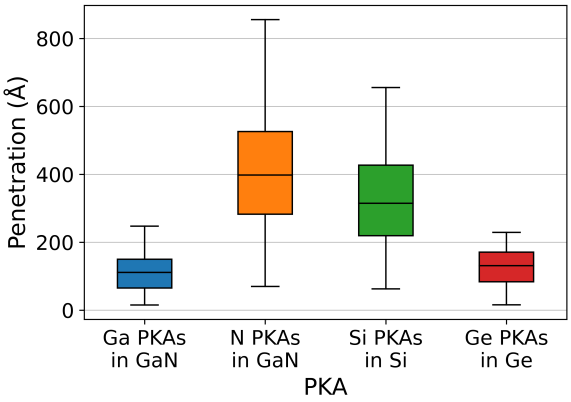

Fig. S2. Box plots of the maximum penetration depth of Ga PKAs in GaN (blue), N PKAs in GaN (orange), Si PKAs in Si (green) and Ge PKAs in Ge (red) for 10 keV collision cascades. From lowest to highest, the horizontal lines of a box plot represent the minimum value of the set, the first quartile value, the median, the third quartile, and the maximum value of the set.

S.II Number of defects

Figures S3 and S4 show the distribution of the number of defects obtained at the end of simulations of 1 keV and 25 keV collision cascades initiated by Ga and N PKAs in GaN, Si PKAs in Si and Ge PKAs in Ge. Large differences between the three materials can be also observed here.

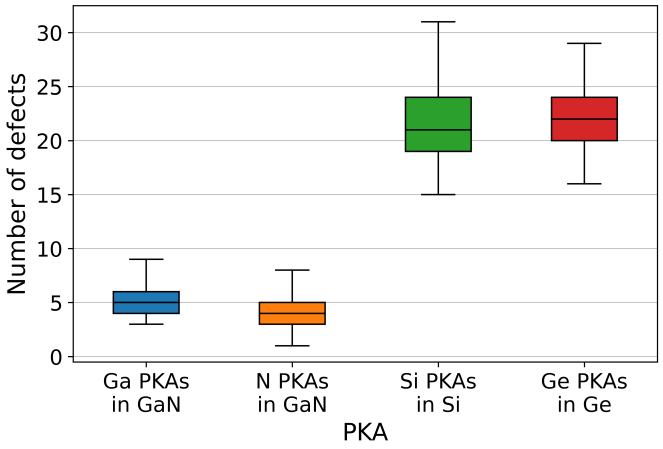

Fig. S3. Box plots of the number of defects after 1 keV collision cascades initiated by Ga PKAs in GAN (blue), N PKAs in GaN (orange), Si PKAs in Si (in green) and Ge PKAs in Ge (in red). From lowest to highest, the horizontal lines of a box plot represent the minimum value of the set, the first quartile value, the median, the third quartile, and the maximum value of the set.

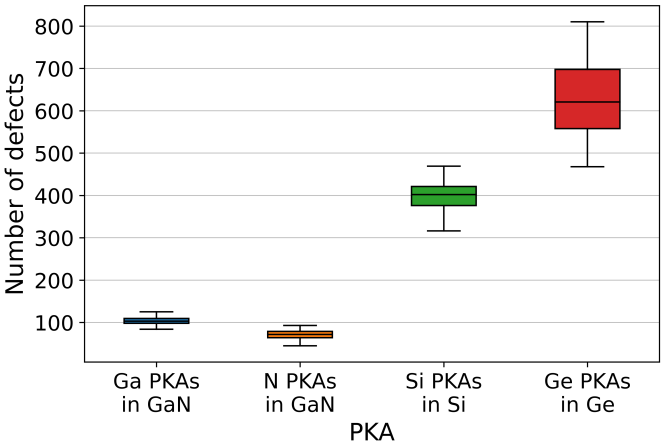

Fig. S4. Box plots of the number of defects after 25 keV collision cascades initiated by Ga PKAs in GAN (blue), N PKAs in GaN (orange), Si PKAs in Si (in green) and Ge PKAs in Ge (in red). From lowest to highest, the horizontal lines of a box plot represent the minimum value of the set, the first quartile value, the median, the third quartile, and the maximum value of the set. One hundred simulations are run for each type of PKA.

S.III Defect number evolution profile

Figures S5 and S6 show the distribution of the number of clusters as a function of their size (number of defects) at the peak of 1 keV and 25 keV collision

cascades and at the end of same collision cascade simulations in GaN (PKAs Ga and N), Si and Ge.

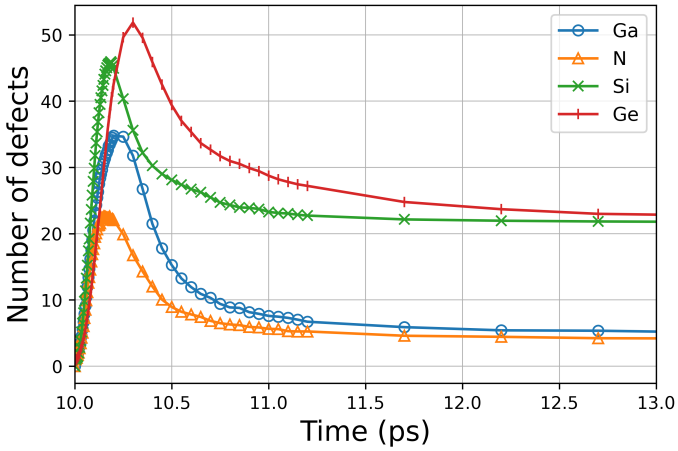

Fig. S5. Defect number evolution profiles during 22 ps for 1 keV collision cascades initiated by Ga PKAs in GaN (blue o), N PKAs in GaN (orange △), Si PKAs in Si (green x) and Ge PKAs in Ge (red |). Defect data are derived from averaging results across 100 simulations for each respective case.

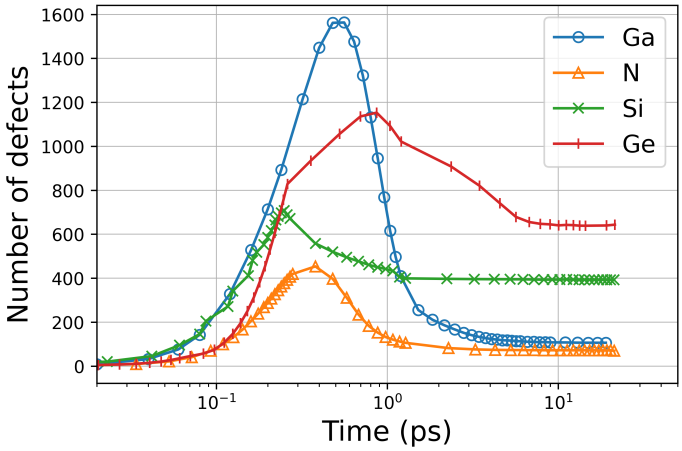

Fig. S6. Defect number evolution profiles during 30 ps for 25 keV collision cascades initiated by Ga PKAs in GaN (blue o), N PKAs in GaN (orange △), Si PKAs in Si (green x) and Ge PKAs in Ge (red |). Defect data are derived from averaging results across 100 simulations for Ga and Ge PKAs, 85 simulations for Si PKAs and 82 simulation for N PKAs.

S.IV Visual representation of defect clusters

Figures S7 and S8 exhibit a visual representation of defect clusters at the peak and at the end of a 1 keV and 25 keV collision cascade simulation, initiated by a Ga PKA in GaN, a N PKA in GaN, a Si PKA in Si and a Ge PKA in Ge. The selected cascades are representative of average cascades for each PKA. They have been chosen because their average penetration depth and average number of defects closely align with the data provided in Table I. Notably, all four cascades share the same direction.

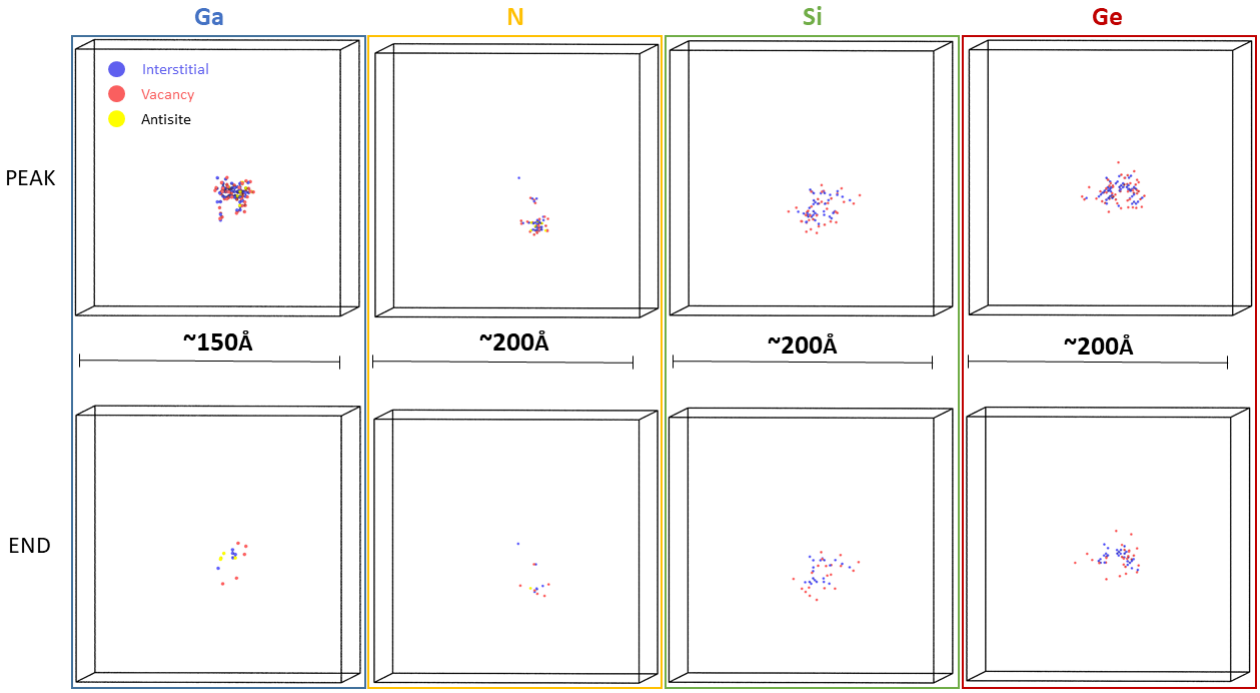

Fig. S7. Visual representation of defect clusters at the peak of a 1 keV collision cascade (top images) and at the end of the same 1 keV collision cascade simulation (bottom images) in GaN (PKAs Ga and N), Si and Ge. The blue spheres represent interstitial atoms, the red spheres represent vacancies and the yellow spheres represent antisites without specifying the type (Ga in an N site or N in a Ga site).

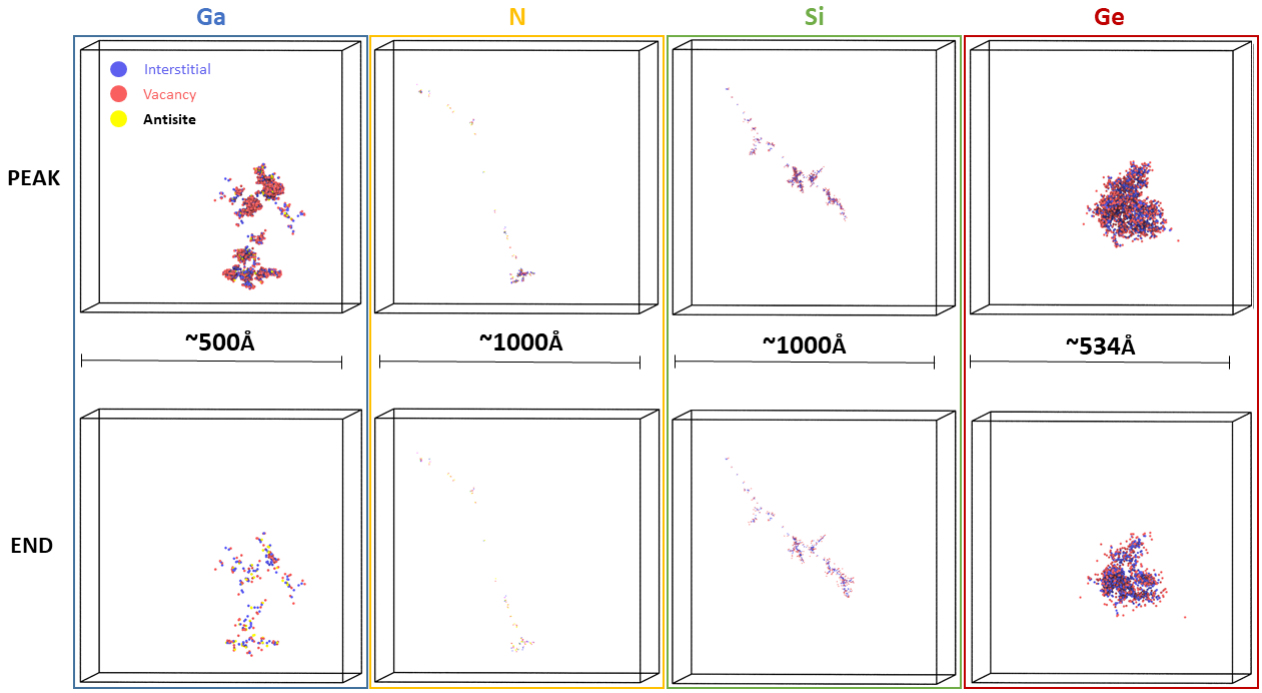

Fig. S8. Visual representation of defect clusters at the peak of a 25 keV collision cascade (top images) and at the end of the same 25 keV collision cascade simulation (bottom images) in GaN (PKAs Ga and N), Si and Ge. The blue spheres represent interstitial atoms, the red spheres represent vacancies and the yellow spheres represent antisites without specifying the type (Ga in an N site or N in a Ga site).

S.V Distribution of the number of clusters as a function of their size

Figures S9 and S10 show the distribution of the number of clusters as a function of their size (number of defects) at the peak of 1 keV and 25 keV collision cascades and at the end of same collision cascade simulations in GaN (PKAs Ga and N), Si and Ge.

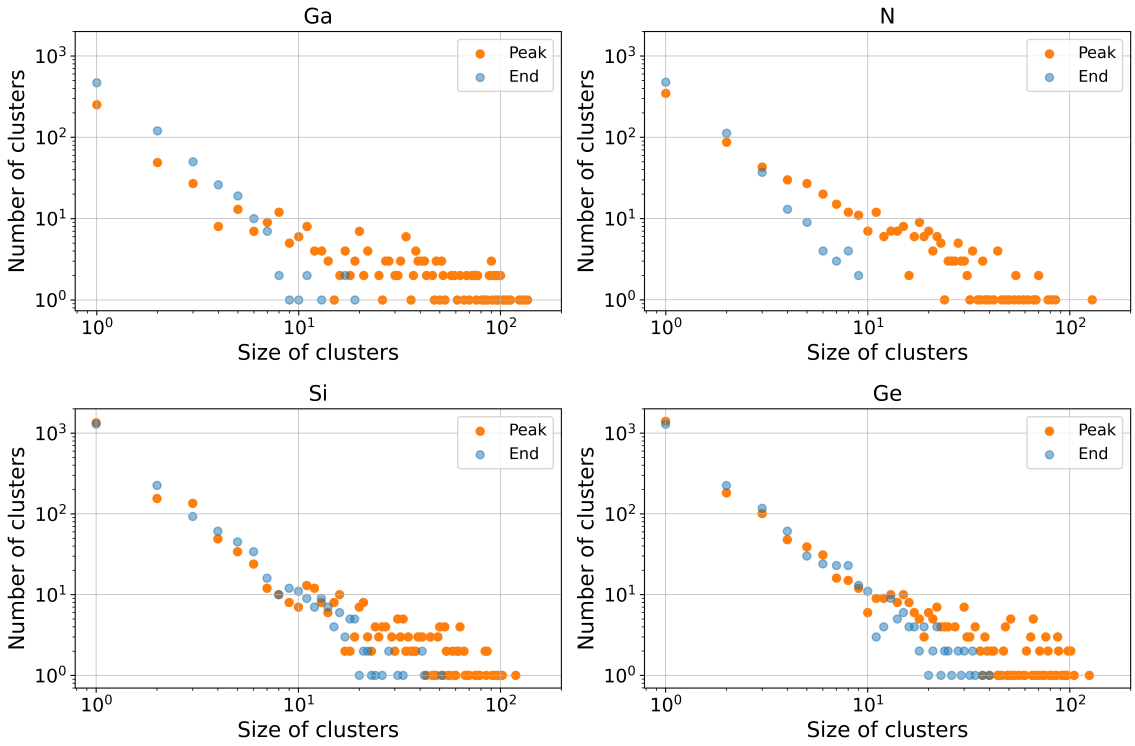

Fig. S9. Distribution of the number of clusters as a function of their size at the peak of the 1 keV collision cascade (orange dots) and at the end of the same collision cascade simulation (blue dots). Ga PKAs in GaN (top left), N PKAs in GaN (top right), Si PKAs in Si (bottom left) and Ge PKAs in Ge (bottom right). Data are obtained from 100 simulations in each case.

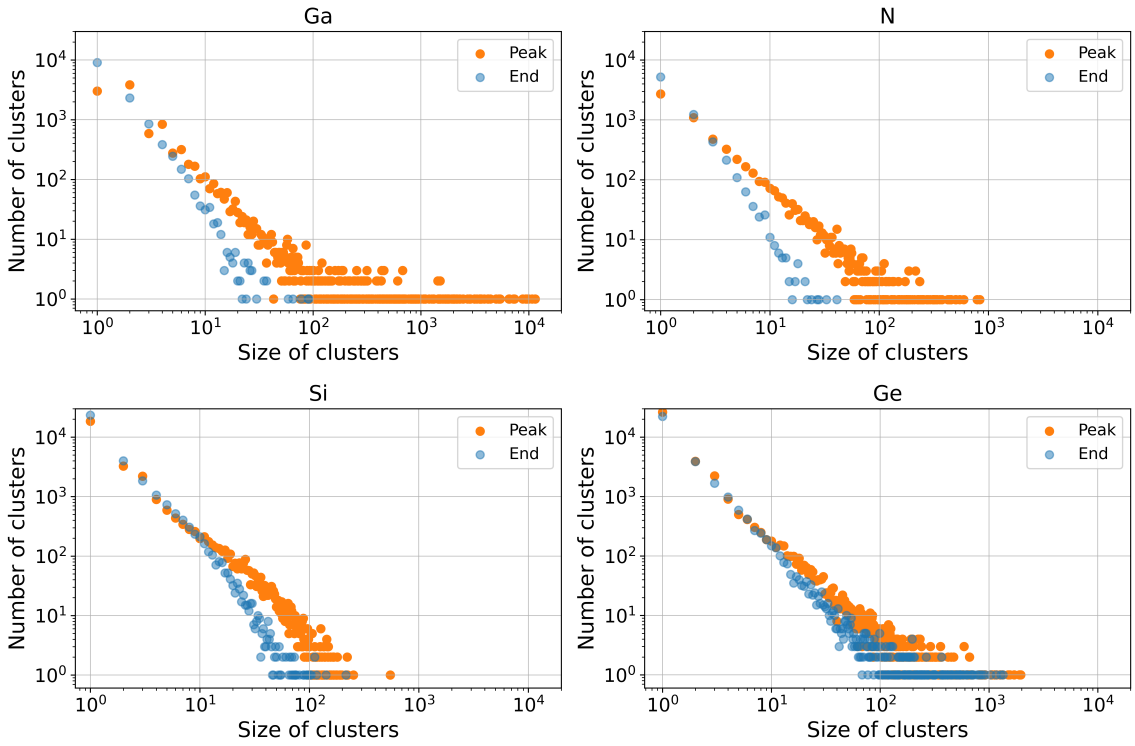

Fig. S10. Distribution of the number of clusters as a function of their size at the peak of the 25 keV collision cascade (orange dots) and at the end of the same collision cascade simulation (blue dots). Ga PKAs in GaN (top left), N PKAs in GaN (top right), Si PKAs in Si (bottom left) and Ge PKAs in Ge (bottom right). Data are obtained from 100 simulations in each case.

S.VI Distribution of interstitial displacement distances

Figures S11 and S12 display the distribution of the distance the interstitials identified at the peak of the cascade (1 keV and 25 keV) are displaced from their initial equilibrium position (called displacement), at the peak of the cascade and at the end of the simulation. Therefore, the displacements plotted at the end are not all coming from interstitial atoms as many of the atoms identified as interstitials at the peak of the cascade are back to their initial position at the end of the simulation.

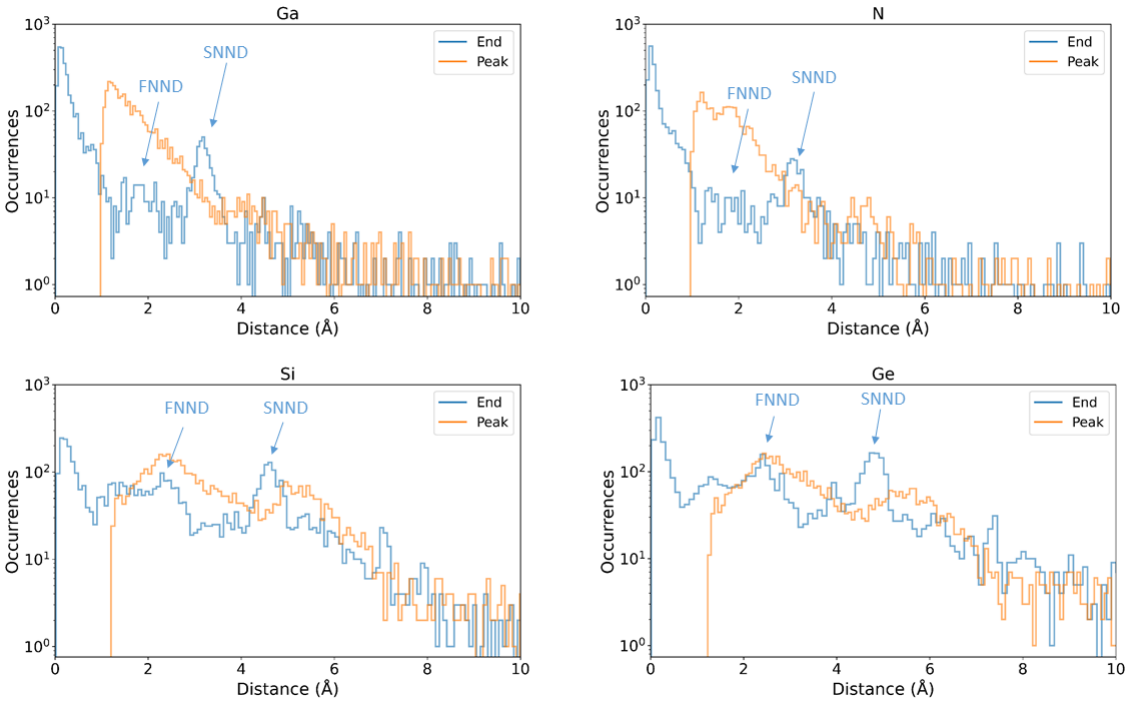

Fig. S11. Distributions of the distance the interstitials identified at the peak of the 1 keV cascades in GaN, Si and Ge are displaced from their initial equilibrium position (called displacement), at the peak of the cascades and at the end of the simulations. The first blue arrow represents the first nearest neighbour distance (FNND), the second represents the second nearest neighbour distance (SNND). Data are obtained from the average of 100 simulations in each case. At the peak of the cascades, the atoms selected to plot the displacements are all interstitials, whereas at the end, atoms identified as interstitials at the peak may have healed back to their initial position, and are thus not interstitials anymore.

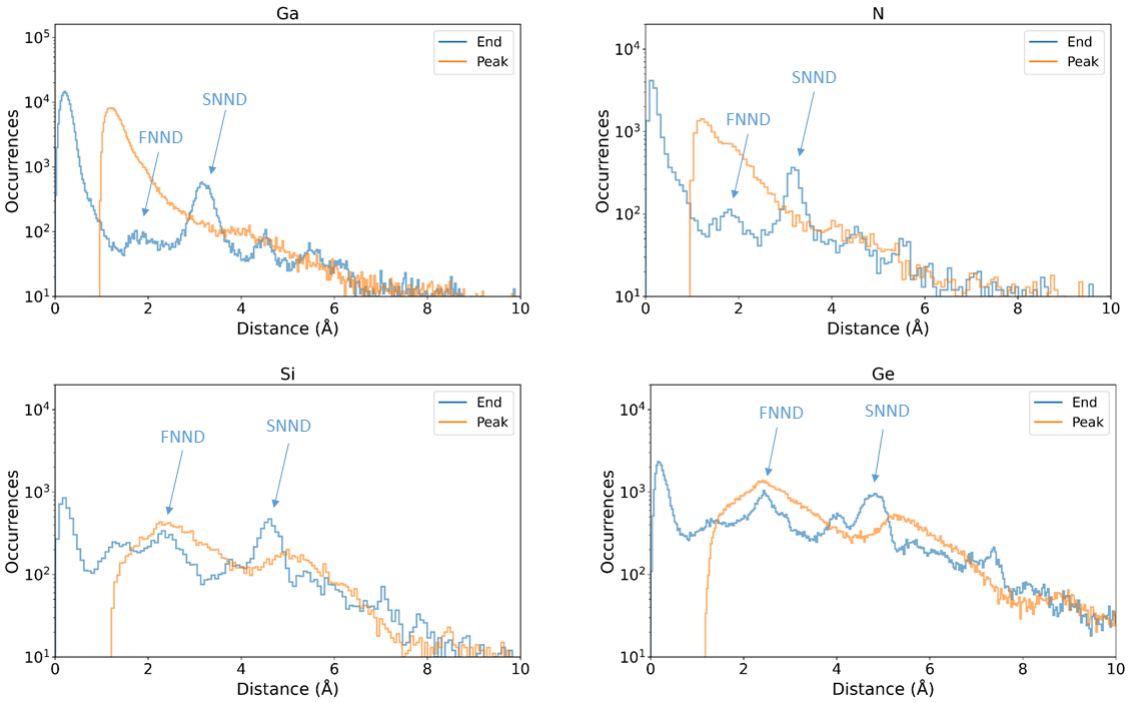

Fig. S12. Distributions of the distance the interstitials identified at the peak of the 25 keV cascades in GaN, Si and Ge are displaced from their initial equilibrium position (called displacement), at the peak of the cascades and at the end of the simulations. The first blue arrow represents the first nearest neighbour distance (FNND), the second represents the second nearest neighbour distance (SNND). Data are obtained from the average of 100 simulations in each case. At the peak of the cascades, the atoms selected to plot the displacements are all interstitials, whereas at the end, atoms identified as interstitials at the peak may have healed back to their initial position, and are thus not interstitials anymore.

S.VII Tersoff/ZBL Potential

To properly describe the equilibrium properties but also the out-of-equilibrium properties, due to the collisions cascades, of the Si, Ge and GaN materials, we combine Tersoff-type potentials $V_{tersoff}$ to the ZBL repulsive potential V_{ZBL}, to end-up with a final potential V_{tot} The potentials are combined in the following way:

$$V_{tot}(r) = F(r)V_{tersoff}(r) + (1 - F(r))V_{ZBL}(r) \quad (1)$$

with a Fermi function $F(r)$ of the following form:

$$F(r) = \frac{1}{1 + e^{-b_F(r-r_F)}} \quad (2)$$

The b_F and r_F parameters for GaN and Si are given in the references in the main text. For Ge, we derived ourselves the parameters ensuring a smooth transisition between the ZBL and Tersoff potentials. The Fermi function parameters we employed for Ge are r_F=0.97 Å and b_F=10.0 Å^{-1}.