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# A detailed approach for the classification and statistical analysis of irradiation induced defects

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ABSTRACT

New criteria are presented for the classification and statistical analysis of defects from irradiation cascades that allow a more detailed description of the diversity of damage, especially amorphous regions. Classical molecular dynamics simulations are used to analyze the damage produced by 2 keV Si recoils annealed at 1000 K for 1 ns. Based on a density grouping criterion of elementary defects (displaced atoms and empty lattice sites) the non-uniformity of local defect density within damage regions is revealed. The density criterion is able to distinguish dense damage regions which evolve independently upon annealing (although they are connected by some defects), while keeping small and compact regions unaltered. Damage regions are classified according to the size, net number of defects and compactness, calculated by averaging the distance among all defects, parameters that have a direct impact on their stability.



## 1. Introduction

Irradiation can generate defects in a crystalline lattice due to the collision of energetic particles with lattice atoms. This may happen during the ion implantation process or due to the working conditions of devices (radiation detectors or devices operating in aerospace or radiative environments). Irradiation induced defects can notably alter device performance, since they are responsible for some detrimental effects such as dopant enhanced diffusion [1], leakage currents [2] or type inversion in radiation detectors [3], and also beneficial, as the photoluminescence of defect clusters in Si [4]. Defects with a large variety of sizes, topologies and different electrical properties coexist within a cascade, which makes extremely complicated to assign an experimental signal to a particular defect, especially without a detailed knowledge of damage characteristics. This is particularly challenging for amorphous regions, which are blamed for trapping electrons destroying the functionality of radiation detectors, but are difficult to characterize [3]. An accurate classification and analysis of defects can clarify the complex damage scenario and contribute to bridge the gap between the microscopic defects and their macroscopic effects.

Molecular dynamics is a suitable tool for the study of damage generation and evolution, as it can capture the temporal and spatial scales of these processes. The small dimensions of some defects make them invisible to some experimental techniques and only detectable by indirect measurements, simulation being the best way to get insight. The random behavior of irradiation induced cascades requires a large collection of data and a statistical analysis to get a meaningful description of defect population. The first step for the analysis of damage is the identification of elementary defects (EDs), i.e., displaced atoms (atoms out of a lattice position) and empty sites (unoccupied lattice sites), using one of the available criteria: the potential energy of atoms [5], the atomic bonding [6], or geometric methods [7–9]. Then, EDs are grouped to define damage regions, usually by means of a *neighborhood* criterion in which neighboring defects are considered to belong to the same group. However this method may lead to artificially large damage regions, identifying as a whole, separated damage regions with only a few defects in common and that actually evolve independently. The common classification of damage by its size is too simplistic, as amorphous regions with similar size show different stabilities upon annealing [10]. The interstitial or vacancy content [9], the distribution of local density [11] and geometry [12], could also play a role on damage stability and properties. This indicates that other parameters, and not only the size, must be taken into account to characterize damage regions.

In this paper we propose some criteria for the identification and classification of damage regions, which can anticipate their evolution upon annealing and explain their different behaviors. This analysis is applied to the damage produced by 100 2 keV Si recoils and annealed at 1000 K for 1 ns, which is in the range of the low dose and weak annealing conditions of some radiation detectors.

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## 2. Simulation scheme

Classical molecular dynamics simulations were performed in LAMMPS [13] using the Tersoff semi-empirical potential [14], smoothly splined to the ZBL repulsive potential [15] for a better description of high-energy short-range interactions. Simulation box is cubic with periodic boundary conditions in all dimensions and large enough (240,064 atoms) to avoid the self-overlapping of cascades. All simulations were done at 0 K to avoid dynamic annealing and zero pressure was maintained by scaling cell dimensions. The time step was automatically adjusted according to the maximum kinetic energy of atoms, within a range from 0.01 to 1 fs.

Si recoils were simulated by assigning 2 keV kinetic energy with random directions to an atom situated at the center of the cell. 100 different recoils were used to get statistics of generated defects. Simulations were considered to be finished when the maximum kinetic energy of any atom averaged for 10,000 time steps was below 1 eV. Then, all atom positions were averaged for other 1000 time steps to remove atom vibrations. The final average positions are compared to those in the initial perfect lattice to identify EDs. Those atoms separated from a lattice site more than 0.125 times the lattice parameter (0.68 Å) are labeled as displaced atoms, and consequently, unoccupied lattice sites are considered empty sites. The cutoff distance to identify neighboring EDs is the first minimum of the radial distribution function of amorphous Si at 300 K.

Generated defects were annealed at 1000 K for 1 ns at zero pressure to allow damage evolution upon a weak thermal treatment. The actual simulation temperature (1100 K) has been calculated to compensate for the overestimation of the melting temperature of Si by the Tersoff potential [16].

## 3. Results and discussion

Elementary defects within a cascade are distributed among a large variety of damage regions. Generally, a *neighborhood* criterion is used to group EDs and to define damage regions: if a defect belongs to a group, its neighboring defects are incorporated to that group, and also the neighbors of these neighbors, and so on. The main drawback of the *neighborhood* criterion is that it may lead to unrealistic very large damage regions, which could even include the full cascade. We have observed that, according to this criterion, separated dense damage regions are often considered as one unique group just because a thin chain of EDs puts them in contact, but they evolve independently upon annealing and lead to different defects. To get a better description of damage we propose a new method, the *density* criterion, which defines damage regions according to the local density of EDs. Using the *neighborhood* classification as a starting point, our method searches for high density zones inside damage regions, by identifying those EDs with at least 7 neighboring EDs, and uses these EDs as seeds to make a subdivision of the regions previously defined by the *neighborhood* criterion. First, neighboring seeds are grouped, and then all EDs belonging to the initial region defined by the *neighborhood* criterion are distributed among the groups of seeds, by assigning each ED to its nearest group of seeds. Our data revealed that a threshold value of 7 neighboring EDs is appropriate to identify variations in local density without leading to an excessive fragmentation. The main goal of the *density* grouping criterion is that it reveals the non-uniformity of the local density and it is able to distinguish dense damage regions which evolve independently, while keeping small and compact regions unaltered.

Two basic parameters can be used to classify damage regions: the *size* (total number of EDs, i.e., displaced atoms plus empty sites), which affects damage stability as large regions are known to be more stable [9]; and the *net* number of EDs (number of displaced atoms minus that of empty sites), which determines whether it is interstitial (positive net) or vacancy (negative net) type damage. Fig. 1a shows the effect of applying the *density* criterion to a large damage region with 366 EDs and net −6, resulting from the *neighborhood* criterion (dashed line). Seven new regions are defined which correspond to the zones with a higher concentrations of EDs. Although the global net is −6, the new regions have different values of nets, some of them even positive. In this example, two large dense regions with negative nets are formed (−7 and −5), while regions with positive or null nets (+4, +2, +1, 0) are smaller and located mainly in the periphery. When diffusion is not predominant, damage annealing consists of local recombination of displaced atoms and empty sites keeping the net value. This is illustrated in Fig. 1b, that shows the remaining EDs after 1000 K anneal for 1 ns, grouped by the *density* criterion. Several of the initial regions have lost a significant number of defects but they are still present, and have a net similar to the as-implanted value.

Insight into the effect of thermal treatments on damage can be got by plotting as-implanted and annealed damage regions according to their size and net. Fig. 2 shows the mean size and number of regions classified by their net, averaged over 100 recoils. As-implanted and annealed damage regions are defined by the *density* criterion; the *neighborhood* criterion is also used for the as-implanted case for comparison. The *density* grouping criterion results in a larger number of as-implanted damage regions (13% increase) with smaller sizes, compared to the *neighborhood* criterion. However, both criteria provide similar results on annealed damage (not shown in this paper) (1% increase with the *density* criterion) as our criterion does not modify small and compact damage regions. As can be seen, there are many small damage regions, with nets between −1 and +1, which mainly correspond to different configurations of point defects. The largest damage regions, usually known as amorphous regions, have negative nets, i.e., they are rich in vacancies. Upon annealing, the general trend is that both the mean number and size of regions is reduced. Some small damage regions are completely annihilated, while bigger ones are reduced in size by recombination or fragmentation. However, there is an increase in the number and size of regions with positive nets (+2, +3). This may be caused by the fragmentation of large amorphous regions and the formation of small regions with positive nets, as a consequence of the non-uniform distribution of density. Interstitial diffusion and interaction could also lead to the formation of small interstitial clusters (positive net). The effect of applying the *density* criterion, when compared to the *neighborhood* classification, is similar to the effect of the annealing. This indicates that the density criterion is somehow able to anticipate the evolution that damage will undergo under a thermal treatment. Note that after annealing only a 36% of the initial damage remains, and applying the *density* criterion is just a different classification of the same amount of as-implanted damage.

Along with size, another parameter that affects the stability of amorphous regions is the geometry, as compact regions survive longer than those with an irregular topology [10–12]. A more accurate and detailed classification of damage should also include the compactness of damage regions, together with the size and the net. We define the compactness of damage regions as the ratio between the average distance among all its EDs, and the average distance of EDs in a spherical region with the same size, used as reference. This is done by calculating the mean distance of each defect to any other defect in the region, and averaging these values over all defects. Fig. 3 shows the compactness of as-implanted damage regions defined by the *density* criterion as a function of size. Point defects and small clusters (size lower than 10) are not included. It is noticeable the large dispersion of the values of compactness even for regions with the same size. As an example of the

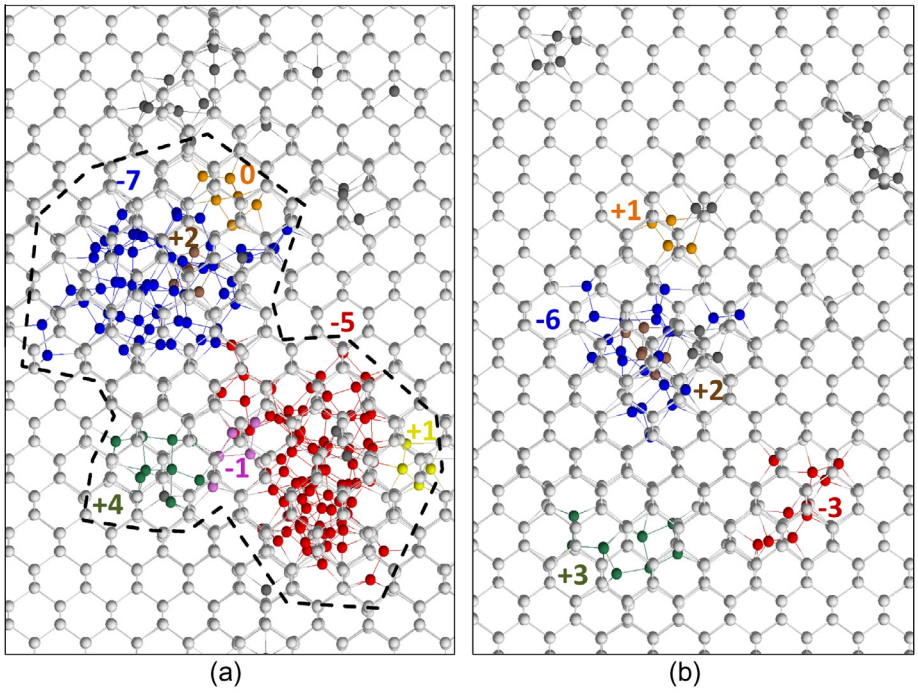


**Fig. 1.** (a) As-implanted damage region (dashed line) containing 366 EDs and a global net of −6, as defined by the *neighborhood* criterion. By applying the *density* criterion seven new regions are defined, plotted in different colors together with their nets. Dark gray atoms represent EDs belonging to other regions; (b) remaining damage regions for the same recoil after 1000 K annealing for 1 ns. The same color indicates that the as-implanted and the annealed regions are related. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

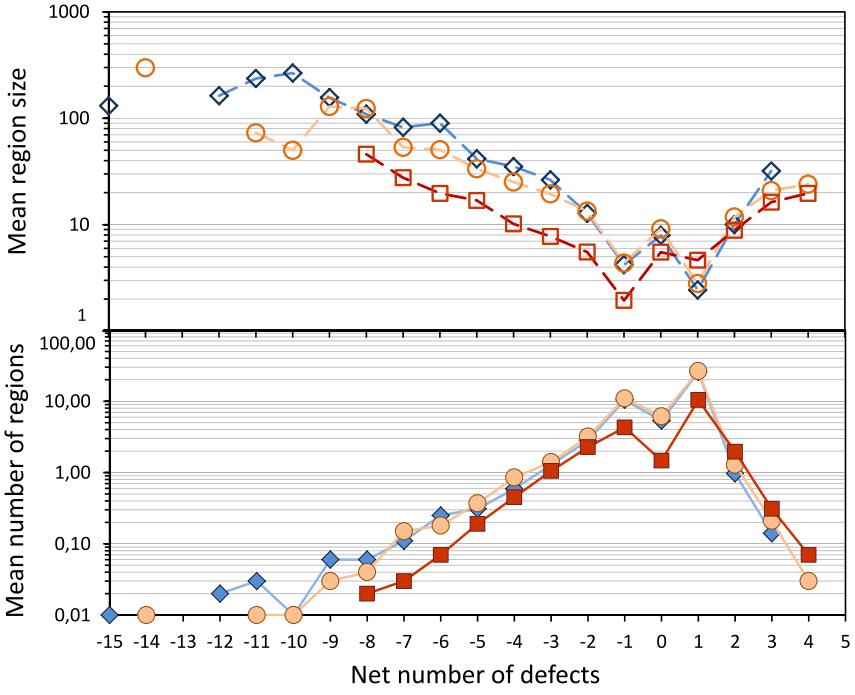


**Fig. 2.** Mean number and size of damage regions as-implanted and after annealing at 1000 K for 1 ns as a function of their net. Solid symbols and lines represent the average number of regions (bottom), while empty symbols and dashed lines show the mean size (top). As-implanted damage is classified by the *neighborhood* criterion (diamonds) and by the *density* criterion (circles). Annealed damage (squares) has been grouped by the *density* criterion.

role of compactness on stability, we show in the inset two as-implanted regions with the same size (39 EDs) and net (−1), but different compactness. Region A is very compact and around 40% of its defects survive annealing, while region B is highly irregular and only a few defects remain.

## 4. Conclusions

The analysis of irradiation induced damage is complicated due to the great diversity of defects that may exist. In this work we present some criteria for the detailed classification and statistical

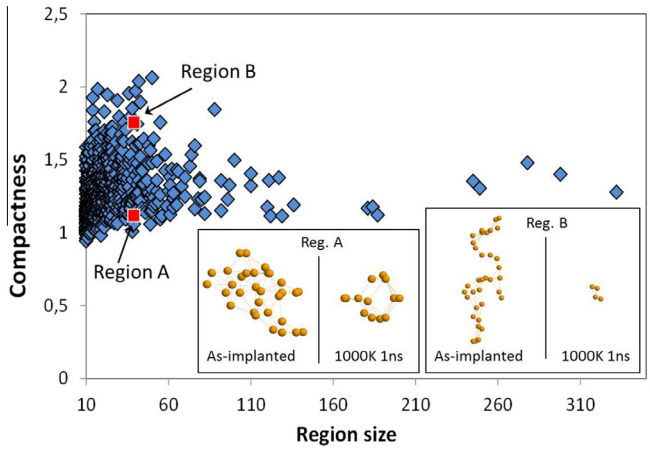


**Fig. 3.** Compactness of as-implanted damage regions (diamonds) as a function of size. The inset is a non-lattice view of two damage regions with the same size (39 EDs) and net (−1), but different compactness (squares). Circles represent both displaced atoms and empty sites belonging to as-implanted and after annealing regions.

analysis of defects. We propose a *density* criterion to identify damage regions, which defines damage regions according to the local density of EDs. This criterion reveals the non-uniformity of local density and it is able to anticipate damage evolution upon annealing, while keeping small and compact regions unaltered. Damage regions are classified by the size, the net and the compactness, calculated by averaging the defect distance in a region. These parameters play a key role on the stability of defects and allow a more accurate classification of damage, which is especially challenging for amorphous regions. The criteria we propose can contribute to unveil the differences among apparently similar amorphous regions, and therefore to clarify how these regions alter device performance.

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