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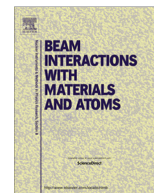

On the origin of dislocation loops in irradiated materials: A point of view from silicon

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ABSTRACT

Numerous dislocation loops are often observed in irradiated and nuclear materials, affecting many physical properties. The understanding of their origin and of their growth mechanism remains unclear rendering all modeling efforts elusive. In this paper, we remind the knowledge which has been gained during the last 20 years on the formation and growth of extrinsic dislocations loops in irradiated/implanted silicon. From the compilation of a large number of experimental results, a unified picture describing the thermal evolution of interstitial defects, from the di-interstitial stable at room temperature, to "magic-size" clusters then to rod-like defects and finally to large dislocation loops of two types has emerged. All these defects grow by Ostwald ripening, i.e. by interchanging the interstitial atoms they are composed of, and transform from one to the other driven by the resulting reduction of the defect formation energy. A model has been proposed and is now integrated into process simulators which quantitatively describes the thermal evolution of all these defects, based on pertinent formation energies. The influence of the proximity of free surfaces or other recombining interfaces can be integrated, allowing simulating the possible dissolution of defects.

It is suggested that, beyond silicon, the same type of scenario may take place in many materials. Dislocation loops are just one, easily detectable among many, type of defects which forms during the growth of self-interstitials. They do not nucleate but result from the growth and transformation of smaller defects.

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1. Introduction

The point defects generated by irradiation in nuclear fuel form extended defects, such as dislocation loops and voids. These extended defects affect the microstructure of the fuel, leading to degradation of its thermal and mechanical properties. Moreover, these defects play an important role in the release of fission gaseous products. In order to fully understand and to be able to accurately predict through modeling the microstructural evolution under irradiation, elucidating the underlying formation mechanisms of these extended defects is important.

There has been much debate in recent years concerning the origin and behavior of the dislocation loops which are observed in uranium dioxide and its surrogates [1]. Two distinct types of extrinsic dislocation loops were observed depending on experimental conditions, both lying on (111) planes but with different Burgers vector $(a/2)\langle 110\rangle$ or $(a/3)\langle 111\rangle$. Efforts to model their nucleation have faced great difficulties; in particular the formation energies of such dislocation loops appear unrealistically too large when they contain only a few atoms. Moreover, their growth mechanism is still unclear.

Having spent the last 20 years working on the characterization and modeling of extended defects in Silicon, we were told of the above situation by colleagues from the nuclear community and struck by the similarities of this situation with the one the silicon community had to face about twenty years ago. Indeed, the same two types of dislocation loops were found in silicon after "irradiation", actually ion implantation, and it took us a while and lots of experiments to understand then model the formation and thermal evolution of these defects. Today, it is understood and physically based models exist, either analytical or based on Monte Carlo methods, which have been implemented in academic and commercial codes aimed at predicting the effect of processes in semiconductors [2–5].

It is thus the goal of this paper to summarize the main results of the work undertaken by the silicon community to describe the formation and evolution of extrinsic (interstitial) defects in silicon. While these materials, silicon and uranium dioxide, are very

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different, we believe that the scenario describing defect evolution in both materials may be quite similar. In particular, we will answer to the following questions, which we have found to summarize the debate animating the nuclear community today:

– Do dislocation loops nucleate from point defects?
– Why are their formation energies unrealistic at small sizes?
– What is the growth mechanism of these loops?
– Why the majority of loops are sometimes observed to be Frank faulted loops and sometimes prismatic (unfaulted) loops?

2. How to form interstitial defects by "irradiation in silicon?

Self-irradiation of course does not exist in silicon. However, there exist different means to generate silicon self-interstitials atoms (Is) which, after annealing, can cluster within extrinsic dislocation loops. Historically, such defects were first observed after high temperature annealing of silicon implanted with dopant atoms. In such cases, the impurity atoms are implanted as interstitials and are activated i.e., locate on substitutional sites, during annealing, ejecting the same number of Si self-interstitials from their original lattice sites. Another simple technique to generate a supersaturation of Is is to directly implant Si^+ ions into silicon, but at sufficiently low doses to prevent the amorphization of the Si crystal to occur [6]. A last technique is to fully amorphize the Si layer by high dose ion implantation with heavy ions such as Ge [7]. In this case, the lattice atoms which are recoiled below the crystalline-amorphous interface accumulate and generate a large supersaturation of Si self-interstitials at this exact location. In these two cases, high temperature annealing leads to the formation of extrinsic dislocations loops.

3. Crystallography of dislocation loops

In general, two types of dislocations are observed (Fig. 1) in different proportions depending on precise experimental conditions. Their characteristics were determined by contrast analysis of TEM images taken under different weak beam conditions and later confirmed by more sophisticated techniques [8,9].

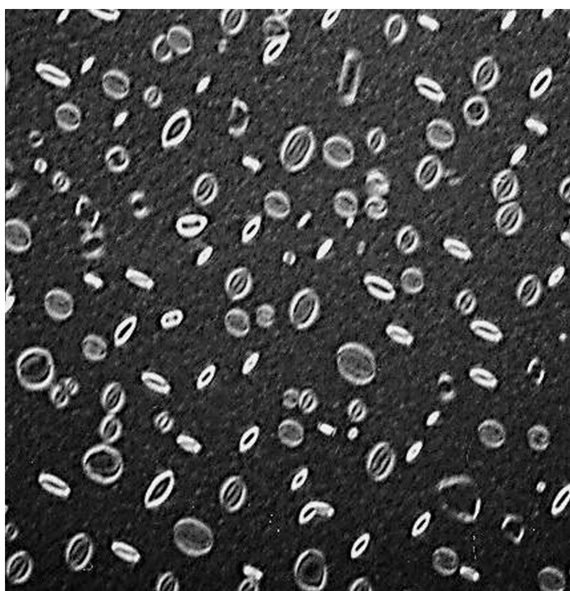

Fig. 1. Typical population of dislocation loops observed by TEM after high temperature annealing (1000 °C, 50 s) of ion implanted silicon (amorphized by Ge, 150 keV, 2×10^{15} ions/cm^2). Two types of dislocations are seen: Frank loops are seen as ellipses, the perfect loops are elongated. Imaging conditions: $\boldsymbol{B} = [001]$, (g, 2g), $g = 004$.

The {1 1 1} faulted circular Frank loops. These loops are interstitial i.e., they are extrinsic defects. As directly seen in the High Resolution TEM image shown in Fig. 2, they consist of two roughly circular extra {1 1 1} net planes of Si atoms, with a stacking fault displacement vector $\boldsymbol{R} = a/3\langle 111\rangle$ and a planar density of interstitials $d = 15.66\ \text{nm}^{-2}$. The fault is bounded by a Frank partial dislocation whose $\boldsymbol{b} = a/3\langle 111\rangle$, i.e. a pure edge dislocation so that this defect cannot glide and can grow only by climb. There are four variants of such loops, each lying on one of the 4 equivalent {1 1 1} planes.

When plane-viewed in a (0 0 1) Si wafer, with $\boldsymbol{B} = [001]$, they project as ellipses whose large axes (i.e. diameters) are parallel to the two perpendicular [1 1 0] and [1 1 0] directions of the foil. Counting the total number of interstitial Si atoms agglomerated within these loops only requires the measurements of these large axes and of the areal loop density.

The {1 1 1} perfect elongated loops. Perfect $a/2\langle 110\rangle$ loops can appear as elongated, more or less circular, or even hexagonal objects. They have {1 1 1} habit planes and are elongated along the $\langle 110\rangle$ directions perpendicular to their $\boldsymbol{b}$. Each (1 1 1) plane containing three $\langle 110\rangle$ directions, there are twelve variants of such defects. The planar density of Is stored within such defects is thought to be the same than within faulted dislocation loops.

It is striking to note that these two types of dislocation loops are exactly the same than those reported to exist in uranium dioxide and its surrogates.

4. Growth mechanism: Ostwald ripening

Fig. 3 shows the evolution of a population of dislocation loops such as the one shown in Fig. 2 during annealing at 1000 °C. After 50 s of annealing, the population consists of a mixture of both types, faulted and perfect, dislocation loops. When the annealing time increases, only the faulted loops survive. Obviously, the dislocation loops appear larger and in smaller densities as the annealing proceeds.

The statistical analysis of large field of view TEM images, taken under appropriate well-defined conditions and taking into account the contrast rules which apply to each of the 16 (12 + 4) crystallographic variants (10), allows to quantitatively follow the growth of these dislocation loops through the evolution of their size histograms. Fig. 4 shows the result of this analysis for the samples annealed at 1000 °C.

Beside the size increase and density decrease of the loop population, it is important to note that the total number of Si atoms stored within these defects stays constant all along this growth process. For this reason, and from the characteristics of the size histograms, we have deduced that the observed growth was due to the interchange of Si atoms between defects of different sizes following an Ostwald ripening process [10], similarly to what is observed for the growth of precipitates in solid matrices (see Fig. 5).

The Ostwald ripening theory was initially developed to describe the growth of a population of water droplets in equilibrium with a supersaturated vapor. At any given temperature, there exists a dynamical equilibrium between a droplet and the vapor surrounding it. The amplitude of this supersaturation only depends on the diameter of the droplet (formally on its curvature radius). This equilibrium is set by the Gibbs–Thomson equation. This theory can be adapted to the case of solid precipitates in a solid matrix and thus, extended to extrinsic defects in silicon [11,12].

Indeed, dislocations loops are just 2D precipitates of silicon atoms in particular orientation relationships within a silicon

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