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From point defects to dislocation loops: A comprehensive modelling framework for self-interstitial defects in silicon

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ABSTRACT

An atomistic model for self-interstitial extended defects is presented in this work. The model is able to predict a wide variety of experimental results by using a limited set of assumptions about the shape and emission frequency of extended defects, and taking as parameters the interstitial binding energies of extended defects versus their size. The model accounts for the whole extended defect evolution, from the initial small irregular clusters to the {3 1 1} defects and to the more stable dislocation loops. It predicts the extended defect dissolution, supersaturation and defect size evolution with time, and it takes into account the thermally activated transformation of {3 1 1} defects into dislocation loops. Moreover, the model is also used to explore a two-phase exponential decay observed in the dissolution of {3 1 1} defects.

1. Introduction

Current technology uses ion implantation as the main process to introduce dopants in silicon. Inherent to this process is the creation of a high amount of point defects, leading to the formation of different defect agglomerates. Their subsequent dissolution during annealing generates a point defect supersaturation that affects the diffusion of the implanted dopants. A thorough understanding of the dissolution kinetics of these defects is needed in order to correctly predict and control the final dopant profile in the deep sub-micron regime. In particular, extra self-interstitials (I) released both from big {3 1 1} rod-like defects [1] and small clusters [2] bring about the transient enhanced diffusion (TED) of commonly used dopants. Four types of self-interstitial extended defects have been detected experimentally in silicon [3]: small irregular clusters, {3 1 1} defects and faulted and perfect dislocation loops (DLs). All of these defects are of extrinsic character, i.e. they are formed with extra Si atoms precipitated as clusters.

The {3 1 1} defect structure, formed by eight-membered atom rings, was first proposed by Takeda [4] for the rod like defects. The role of {3 1 1} defects in the TED of boron was proposed by Eaglesham et al. [1], demonstrating a correlation between the number of interstitials emitted by the defects and the flux of interstitials driving TED, and the importance of the surface for the {3 1 1} defect dissolution. A study about the smaller precursor clusters that nucleate and grow into {3 1 1}'s was reported by Cowern et al. [5], showing that these small clusters also contribute to the TED, and their binding energies exhibit dramatic fluctuations for small sizes. Experiments on the {3 1 1} defect size evolution with time [6] concluded that the {3 1 1} defect dissolution did not seem to be controlled by the surface recombination rate. Quantitative TEM studies on the depth profile of {3 1 1} defects [7] found that the defect band dissolves preferentially at the surface side, in apparent contradiction with Ref. [6]. This apparent contradiction was solved both theoretically [8,9] and experimentally [7]. The ripening and dissolution of Si extended defects is not produced by one single cause, but it is a competition between the surface and other defects to capture the interstitials. Finally [9,10] two different regimes were found during the evolution of {3 1 1} defects, a weakly non-conservative Ostwald ripening phase followed by a very rapid defect dissolution.

DLs are planar defects lying on {1 1 1} planes [11] and can be either faulted loops (FDL) or perfect loops (PDL). FDLs consist of a circular stacking fault surrounded by a dislocation line. PDLs have an extra plane of atoms instead of the stacking fault. Based on experimental observations [12] the unfaulting of the {3 1 1} defects is the source of the subthreshold DLs in non-amorphized ion-implanted silicon, i.e. the {3 1 1} defects can either dissolve or unfault into loops.

The total TED (i.e. the final dopant diffusion after the complete annealing of interstitial defects) depends mainly on the amount of

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excess interstitials (approximately accounted by the "+n" model) [13,14] and on the depth at which the defects are formed. Therefore, to predict the total TED it is not critical to know the time evolution of self-interstitial supersaturation. However, for the case of incomplete anneals (whereby extended {3 1 1} defects or DLs still remain) the transient of self-interstitial supersaturation will be critical. This interstitial supersaturation is related to the energetics of the interstitial defects and defects present in the sample [15,5]. Consequently to correctly account for TED for incomplete anneals, process simulators have to implement predictive models for the evolution of the small clusters, {3 1 1} defects and DLs. In particular, the formation of (stable) DLs decreases the supersaturation by several orders of magnitude and it will severely affect the dopant profiles after the incomplete annealing. In this case, the dopant profile would be expected to be shallower but the structural quality of the sample will be affected. In consequence, the modelling and accurate prediction of the transition from {3 1 1} defects to DLs is imperative.

A considerable effort, using both continuum [5,8,10,16–20] and atomistic [9,21] approaches, has been devoted to the understanding of the physical mechanisms that control the nucleation, growth and dissolution of extended defects. The continuum method however, is limited by the number of equations that can be solved without running into prohibitive CPU demands and/or convergence instabilities. Moreover, it uses some simplifying assumptions about the capture volume, and it makes a continuum treatment of the (discrete) extended defects.

In this work, we have developed a comprehensive atomistic extended defect model which accounts for the whole defect evolution: the point defects nucleate into small clusters which will transform into {3 1 1} defects which finally can become DLs. The model has been implemented in Sentaurus Process KMC [22], which uses the kinetic Monte Carlo (kMC) technique [23]. This model uses one single set of parameters to explain all the different simulation conditions.

2. Physical model

In our model I_s and V_s are represented as points in a 3D simulation domain (see Fig. 1), and they are given random jumps at a rate derived from their diffusivities. They can interact with other particles which are found within their capture radius, leading to cluster formation or recombination [23]. The jump distance and the capture radius is always assumed to be the second neighbor's distance in the silicon lattice.

2.1. Shape

Our model assumes the shape of interstitial clusters with size less than 15 interstitials to be irregular. For bigger sizes we rearrange them into the {3 1 1} defects and/or faulted DLs according to the crystalline geometry data. The experimental transition size between small clusters and {3 1 1} defects is not well known, and the literature establishes a size of $n = 10$ as a minimum [5,19] (for lower values there are big variations in the cluster binding energy, as shown in Ref. [5]) and $n = 40$ as a maximum (considered to be the smallest defect that TEM can resolve) [10].

We assume that irregular clusters retain captured point defects at their arrival position. This assumption leads naturally to a roughly spherical shape. On the other hand {3 1 1} defects are modelled as parallel stripes (rows) of interstitials lying in one of the twelve, randomly chosen, orientationsof a {3 1 1} plane. We model the {3 1 1} defect shape, following the experimental data [4], as N_{row} rows of *I*s lying on a $\langle 0\,1\,\bar{1}\rangle$ line with a distance of $a/\sqrt{2}$ between I_s in the same line and N_{col} columns keeping a distance of $a\sqrt{22}/4$ between them, being $a = 0.543$ nm the silicon lattice parameter. We assume that the ratio between length (L) and width (W) is given by [25,8]

$$W \approx \sqrt{CL}, \tag{1}$$

with $C = 0.5$ nm. Consequently, the length of the defects is

$$L \approx 0.5\, n^{2/3} \text{ nm}, \tag{2}$$

n being the defect size. In our model, {3 1 1} defects capture any point defect jumping into the capture volume of the particles belonging to the defect (see Fig. 2). After the capture, the number of N_{col} and N_{row} is recalculated, with a small hysteresis to prevent {3 1 1} defect reshape due to the emission and capture of the same particle. Once the new geometry is computed, the particle is moved to the nearest end of the {3 1 1} defect.

The transformation of {3 1 1} defects into DLs depends on the size of the {3 1 1} defects and on the temperature. DL are expected

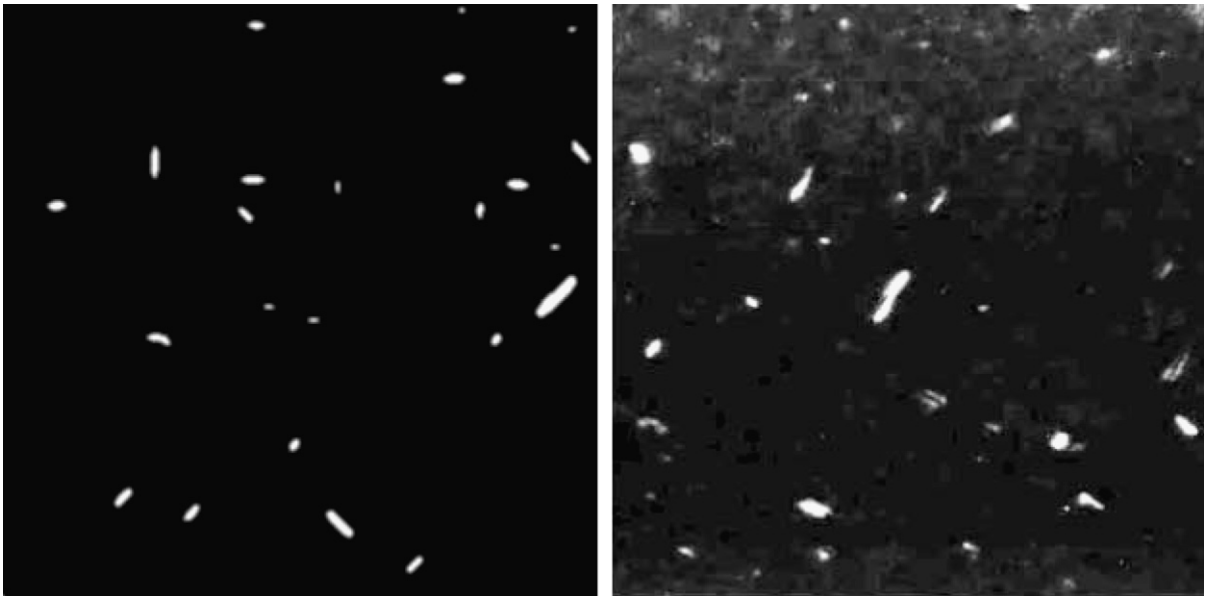

Fig. 1. Left, atomistic view of a simulation after a 5×10^{13} cm^{-2}, 40 keV Si implant, followed by RTA at 815 °C for 30 s. Right, experimental results for these same conditions, taken from Ref. [24].