Relation between thermal evolution of interstitial defects and transient enhanced diffusion in silicon

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Extrinsic defects are often found after ion implantation and annealing of silicon. These defects, which can be detected by Transmission Electron Microscopy (TEM), range from small clusters of unknown structure to the famous {113}'s and to dislocation loops of two types. While all these defects have been observed since decades after specific implantation and annealing conditions, an unified picture explaining why they are observed after such conditions was still lacking. Recent efforts in this direction have been rendered possible because of the need to achieve an understanding of the diffusion anomalies experienced by most dopants in silicon in presence of these defects.

This work reviews the structure and energetics of the most often found extended defects in sillicon and describes the mechanisms by which all these defects grow in size and transform during annealing. We show that these defects grow by interchanging the Si atoms they are composed of, similarly to a classical Ostwald ripening phenomenon driving the growth of precipitates. From di-insterstitials stable at room temperature they evolve into very stable clusters of "magic" sizes composed of 4 and 8 atoms then transform into rod-like defects elongated in <011> directions, the {113} defects. This process can be conservative or not depending on the eventual presence of a strong sink such as a recombining surface in the vicinity of the defects. When the process is conservative the {113}'s do not dissolve but transform into either perfect or faulted dislocation loops. Later on, the two types of loops compete during growth until only the most stable form survives annealing.

Recent experiments (size invariance, surface influence etc...) are presented which definetely prove that the Ostwald ripening is the only mechanism responsible for the growth of all these defects.

The driving force for such an evolution is the reduction of the formation energy of the defects as they grow in size and/or evolve in type. Fig. 1 is a plot showing the variation of the formation energies (E_f) of all these defects as the number of Si atoms they are composed of increases. The clusters' formation energies are from the experimental work of Cowern et al. (1) while that of the {113}'s and of the dislocation loops are obtained by derivating the total energy of the defects (2). From this figure one can understand that a large {113} defect is a sink for the Si atoms emitted by clusters but a source of Si for dislocation loops.

In the mean time, large supersaturations of free Si interstitials (Ci/Ci*) exist in the region, due to the dynamical equilibrium of point defects with extrinsic defects, the amplitude of which is given by the Gibbs-Thomson equation $Ci/Ci^*=\exp(E_f/kT)$. The hierarchy in terms of defect energy induces an even stronger hierarchy of levels of Si supersaturations in the defect region which is at the origin of the transient diffusion anomalies that most dopants encompass during annealing. In the case of boron which diffuses by pairing with Si interstitials, the diffusivity enhancement boron experiences at 800°C can range from 10^5 in presence of clusters to 10^3 in presence of large {113}'s down to 5-3 in presence of dislocation loops.

Finally, we present a physically based model of the growth of extended defects which describes the non-conservative Ostwald ripening of defects in presence of a recombining surface. The defects emit Si atoms at rates that depend on their formation energies and capture them from the mean supersaturation mean-field. We have tested the model against some published experimental studies of TED and defect evolution. It is, for example, shown that the famous dissolution of the {113} defects as reported by Eaglesham et al. (3) is not an intrisic characteristics of the defects but results from a lucky combination of experimental parameters. The model well reproduces all the experiments reported so far concerning both defect kinetics and measured diffusivity enhancements. In particular, after low energy implantation, the surface of the wafer may recombine large amounts of free Si interstitials, driving clusters into dissolution before transformation into more stable forms, eventually detectable by TEM. Consequently, for a typical 1 keV B implant, TED occurs as a short "pulse" at the very beginning of the anneal. In most practical cases, it is found that both defect dissolution and TED are over during the ramping up of the annealing (see Fig. 2).

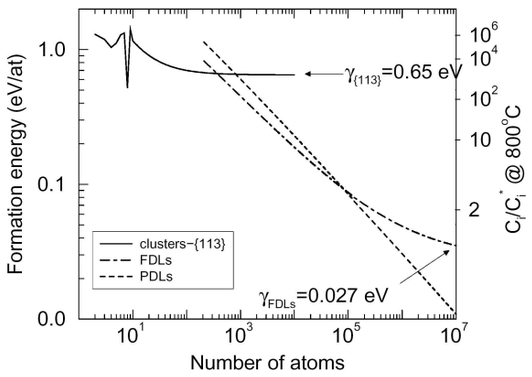

Figure 1: Formation energy (left axis) of the different types of extrinsic defects as a function of their size and corresponding values of the Si(int)s supersaturation (right axis).

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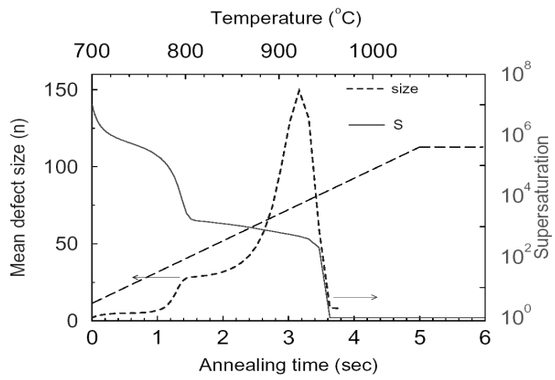

Fig. 2: Evolution of the defect size (dotted) and interstitial supersaturation as a function of annealing time during a typical temperature ramp up.

References

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