# Control of Point Defects, Impurities and Extended Defects in CZ Si: The Original/Ongoing Silicon Nanoscale Defect Engineering

*George A. Rozgonyi*
*Materials Science and Engineering Department,*
North Carolina State University, Raleigh, NC 27695

The formation, interaction, diffusion, and clustering of defect elements in ultra high purity silicon is a key issue in the development of microelectronic device manufacturing and crystal growth methods, as well as with recent nano-scale materials physics phenomenon. As an aid in discussing the range of physical phenomena to be emphasized in this review, we present in Fig. 1 a schematic representation of how the interaction of native point defects with impurities, dopants, and process ambients is coupled to device yield on large diameter silicon wafers via specific extended defects and precipitates. We start our discussion with impurities, see top of Fig. 1, which are conveniently separated into two groups according to their level of chemical and electrical activity within the silicon host lattice. Thus, we have metallic impurities on the left, which are fast diffusing and, particularly for iron, are always considered deleterious to devices, even at concentrations of $10^{10}$cm$^{-3}$. Whereas the group including oxygen, carbon, and nitrogen impurities on the right play a more complex "good guy/bad guy" role with regard to devices, based in large measure upon their propensity for forming silicon oxide based precipitates. These precipitates function either as electron/hole recombination centers, particularly bad for high voltage and photovoltaic devices, or as beneficial gettering centers which reduce the unwanted metallic impurities. Much of the challenge in silicon substrate technology for the past 25 years has been, and continues to be, in creating oxide precipitates with a uniform size and density and positioning them just below a defect-free, metallic impurity-free, denuded zone dedicated to device functions. Although this internal oxidation/impurity trapping process, known as intrinsic gettering, occurs spontaneously during conventional Czochralski wafer thermal sequences, it is strongly coupled to the local balance of vacancies and interstitials, as well as the presence of carbon or nitrogen.

Somewhat more specifically in Fig. 1 we note in the inner annular ring that vacancies, self interstitials, and interstitial oxygen lead to the formation of a group of extended defects highlighted within individual ellipses as precipitate, dislocation loop, stacking fault, and void. These are the micro-scale features that can be delineated by a variety of wafer-scale diagnostic tools and then correlated with individual device properties. Their interdependence is due largely to the near doubling of the volume of an oxide precipitate over that of the host silicon lattice. This produces stress relieving dislocation loops as well as a local flux of interstitials, which form extrinsic stacking faults. In addition, because of their negative impact on gate oxide integrity, recent interest has focused on the condensation of vacancies during crystal growth into octahedra voids, commonly observed as crystal originated pits(COPs). Thus, in this report our primary materials science objective is to examine how vacancies and self interstitials initially complex with oxygen(or nitrogen) to from nanoscale aggregates which either become silicon oxide precipitates or COPS. A secondary and more practical nano-scale defect engineering goal is to review the options for controllably manipulating point defects and impurities via novel dopant and/or thermal processing for 300mm and larger substrates.

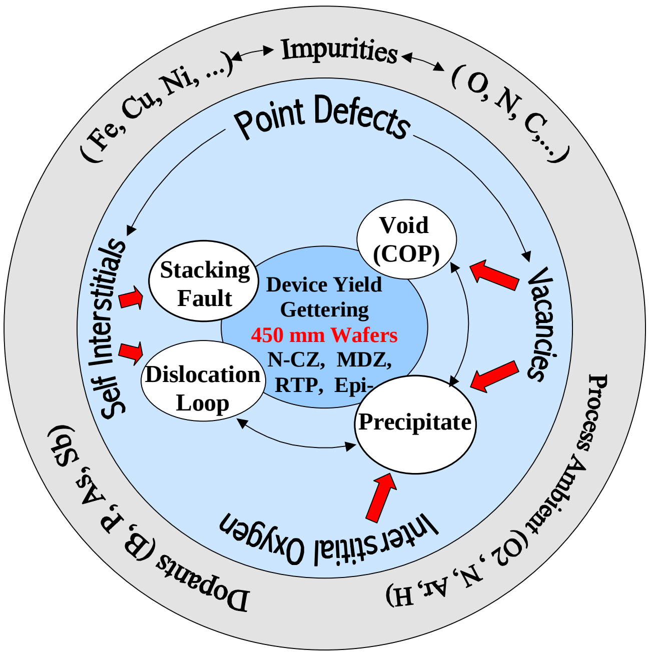

Fig.1 Global Model for Interaction of Point Defects, Impurities, and Extended Defects in CZ Silicon

Recently two basic and fundamentally different approaches to using point defects to control oxygen precipitation have appeared, see papers in [1,2]. Both procedures depend on the fact that, although the concentration of oxygen is more than three orders higher than that of vacancies, it is actually the vacancy concentration that enables one to control the oxygen precipitation. In the first approach, nitrogen doping during crystal growth (N-CZ), at a level comparable to the vacancy concentration, is used to create N-V complexes which serve to simultaneously reduce the size and density of voids and to enhance the nucleation of oxygen precipitates[3]. The second approach, called the MDZ or magic denuded zone process, operates on individual wafers via the rather elegant installation of a depth-dependent, oxygen precipitation controlling, vacancy profile. This process uses an ~1200C RTP anneal to erase the defect history of the as- grown ingot. Whether N-CZ or MDZ wafers are eventually adopted by the IC device community remains to be seen. One thing that is certain, however, is that for 450mm crystals the required materials science understanding for each will be greatly enhanced by efforts to develop accurate computer models and simulations to predict the point defect behavior such that nanoscale defect engineering options are optimized.

1. GADEST 2001, E. Raineri, et al (Eds.), Solid State Phenomena, Vols. 82-84, Trans Tech Pub. Enfield, NH
2. Shonan Forum on Silicon Materials 2001, Yamada-Kaneta and Sumino (Eds.), JTIS, Tokyo, Japan
3. K. Nakai, et al, J. Appl. Phys., **89**, 4301(2001)
4. R. Falster and V.V. Voronkov, Materials Science and Engineering, **B73**, 87(2000)