Analysis of the nucleation kinetics of oxide precipitates in Czochralski silicon

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Although oxide precipitation in Czochralski (CZ) silicon is investigated since decades, it is still not fully understood. This however is prerequisite for accurate modeling of precipitate generation during thermal processes of device fabrication and the creation of getter sites for metal impurities. A few years ago, the so-called magic denuded zone process was discovered which offers the possibility to establish well defined vacancy concentrations in silicon wafers by RTA treatments. This is of great advantage for the investigation of the influence of vacancies on oxide precipitation more into detail. The aim of this work is to study the impact of vacancies on the nucleation of oxide precipitates in order to obtain deeper understanding of the type of nuclei and nucleation sites with their impact on the nucleation kinetics.

We have used moderately boron doped silicon wafers with an interstitial oxygen concentration of 6.4-6.5×10¹⁷ cm⁻³. These wafers received an RTA pretreatment in order to establish certain vacancy concentrations in the wafers depending on the RTA temperature. Subsequently, the wafers obtained a nucleation anneal for 8h at a temperature in the range between 400°C and 1000°C followed by a stabilization anneal at 780°C for 3h and a growth anneal at 1000°C for 16h. The stabilization anneal was omitted for nucleation anneals above 750°C. Bulk microdefect (BMD) density and loss of interstitial oxygen were measured.

Fig. 1 provides examples of the nucleation curves obtained from the BMD measurements. Four peaks can be observed. Two of them appear also without an RTA pretreatment [1, 2]. They have been explained by coherent mono-layered and double-layered agglomeration of oxygen atoms [3]. These peaks increase with increasing vacancy concentration. The two new peaks exhibit a much stronger increase with increasing vacancy concentration. They can be explained with coherent mono-layered and double-layered VO₂ agglomerates. Their features were determined by ab initio calculation using local density approximation of local plane waves. With these four species, a good fit of experimental data can be obtained.

It is also interesting to note that if the temperature of the RTA pretreatment is high enough there is still considerable nucleation even at 1000°C. Until now, this temperature was regarded as a pure growth temperature of oxide precipitates. Another interesting result is that at high vacancy concentration there is also considerable nucleation at 780°C. Halting at this temperature would not serve for stabilization only it also generates additional nuclei. All these issues will be addressed in this contribution.

From theoretical analysis of the results, we obtained quite clear evidence that modeling of oxide precipitation should be done with the enhanced effective diffusivity as it is usually obtained from out-diffusion [4] and precipitation [5] measurements but not as it is obtained from dislocation unlocking experiments [6]. The appropriate formulas for modeling the effective diffusivity are developed from experimental data in the literature. Precise FTIR measurements of the oxygen dimer and trimer absorption with improved sensitivity confirm that the concentration of oxygen dimers is in deed in the range of 10¹⁵-10¹⁶ cm⁻³ as it is found in out-diffusion and precipitation experiments.

Very interesting results were obtained from the analysis of the density of nucleation sites and from the time dependence of the nucleation rate. In the temperature range from 450°C to 700°C, the nucleation rate increases until it saturates after a few hours. Below and above this temperature, the nucleation rate decreases with...
time until it remains constant after a few hours. This behavior can be explained by generation and dissolution kinetics of the nucleation sites. Analysis of nucleation within this model which is based on classical nucleation theory has shown that the nucleation of oxide precipitates takes place at heterogeneous nucleation sites. These sites contain oxygen atoms and vacancies. One type of sites is stable between 450°C and 700°C. It is decaying at higher temperature. A detailed analysis of the nucleation sites will be presented.

In summary, from the nucleation experiments with well defined vacancy concentrations new insight into the oxide precipitation process was obtained and new approaches for modeling were developed [7].

![Figure 1: Nucleation rate after RTA pretreatments at 1225, 1175, and 1100 °C for 30s [7].](image)

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REFERENCES