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Modeling and Simulation of Oxygen Precipitation in Si: Precipitate–Point Defect Interactions and Influence of Hydrogen

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Since the oxygen content of Czochralski-silicon wafers usually exceeds the solid-solubility limit at temperatures used in ULSI fabrication processes, oxygen precipitates are formed during the thermal treatments. Precipitation is usually accompanied by secondary defects such as stacking faults and dislocation loops. While oxygen precipitates and/or precipitate-dislocation complexes act as gettering sites for unwanted metallic impurities, the mechanical strength of Si-wafers decreases with increasing oxygen precipitation. Another important effect of oxygen induced defect is their influence on gate oxide integrity (GOI). It is well known that GOI is strongly dependent on silicon wafer quality of the near-surface/surface region. If the wafer has an insufficent defect-free zone (denuded zone), the GOI and accordingly the dielectric breakdown of thin gate oxides worsen drastically. From the viewpoints of gettering efficiency, mechanical strength, and GOI, it is, therefore, necessary to optimize oxygen precipitation, which strongly depends on thermal treatment conditions, initial oxygen concentration, and crystal quality.

Most of the precipitation models reported during the last two decades are based mainly on the classical nucleation theory. The major deficiency of these models is that they are not able to describe the loss of oxygen and the change of total precipitate density consistently. Furthermore, they do not consider precipitate–point defect interactions and formation of stacking faults.

In this work we present recent model developments based on our previous model [1], which describes the precipitation of oxygen and the formation of stacking faults simultaneously using rate– and Fokker–Planck equations. We have improved the model to consider the influence of vacancies on precipitation in addition that of self interstitials. A partitioning between vacancies and self interstitials is obtained by assuming that the system always seeks its minimum energy configuration. In Figure 1 the number of absorbed vacancies x, the number of emitted self interstitials y, and the residual precipitate strain δ are shown as function of the super/undersaturation of self interstitials and vacancies, S_I and S_V, respectively. Depending on point defect concentrations at the far field of diffusion both vacancies and self interstitials take part in the precipitation process. The residual strain is, then, determined by point defect interactions.

One of the recent achievements to improve the surface quality is to anneal the wafers at high temperatures in hydrogen ambient. Though the mechanism, how hydrogen influences the behavior of oxygen, is still highly controversial, it is a common experimental observation that hydrogen annealed wafers have better GOI and deeper denuded zone than those annealed in neutral ambients. In this work we additionally report our attempt to model the influence of hydrogen on oxygen precipitation. By means of oxygen outdiffusion profiles of hydrogen annealed wafers we could obtain a relationship for the temperature dependence of the

oxygen concentration at the wafer surface. Using this relation we have found very good agreement between experimental [2] and simulated results. Figure 2 shows the precipitate density as a function of wafer depth after two different 3-step annealings. In the near-surface region hydrogen annealing results in less precipitate formation (broken line) than in neutral ambient (solid line). In Figure 3 the precipitate size distribution after the 3rd step is plotted as a function of precipitate size and wafer depth. From the figure one can clearly see the denuded zone. The figure also shows that the bulk is rich of big precipitates, which are indispensible to obtain effective gettering.

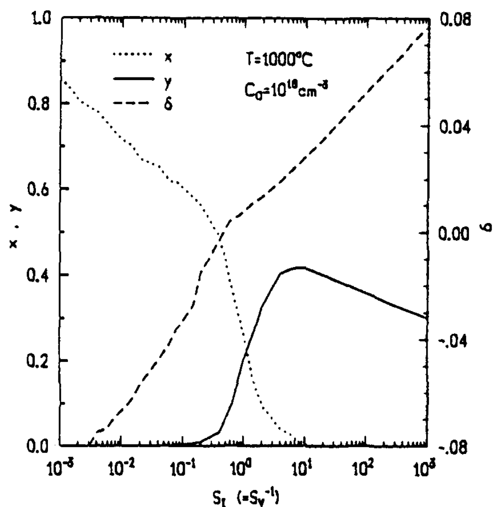


Figure 1:

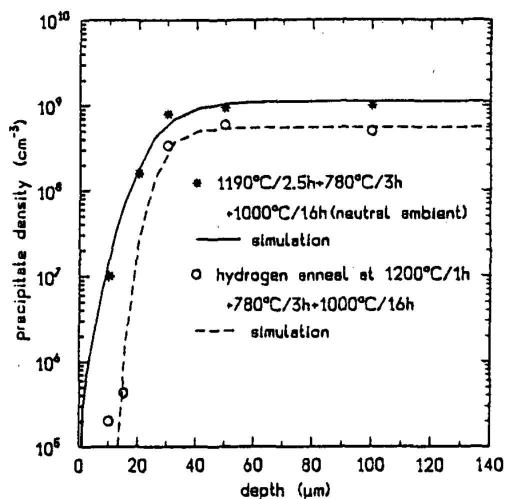
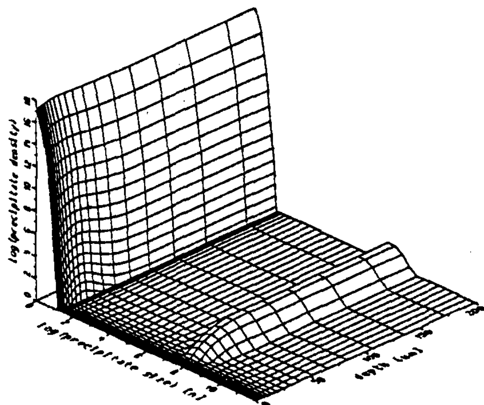


Figure 2:



[1] S. Senkader, J. Esfandyari, and G. Hobler, J. Appl. Phys. 78, 6469 (1995).

[2] H. Kubota, M. Numano, T. Amai, M. Miyashita, S. Samata, and Y. Matsushita, in Semiconductor Silicon/1994, The Electrochem. Soc., Inc., Pennington, NJ., p. 225 (1994).