Cu Gettering Studies in Silicon

Personnel

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SiWEDs

We are conducting gettering experiments to verify the models used in our simulator and to better model other important mechanisms that ultimately will need to be included in a quantitative processing simulator. We have extended our quantitative model of doping enhanced solubility for Fe in p-type Si to Cu and present those results. Our preliminary experimental results on the study of Cu gettering kinetics in p-type epitaxial wafers that have been in-diffused with Cu from the wafer backside and then quenched demonstrate support for the doping enhancement model. PhotoLuminescence spectroscopy (PL) carried out on the front surface of epitaxial wafers that have been in-diffused at both 950˚C and 450˚C with Cu produced no Cu signal, however FZ wafers of comparable resistivity to the epitaxial layers demonstrated strong Cu peaks after a drive-in at 950C and quench treatment. Step-etching of the Cu treated epitaxial wafers reveals haze below the epi/substrate interface.

Segregation Model

Solubility enhancement of Fe in p-type Si occurs by two mechanisms. One is by the ionization reaction of Fei being driven forward due to the increase in hole concentration and the second is by pairing of Fei^+ to oppositely charged ionized dopants. For the case of Cu in Si, it is estimated that doping does not significantly affect ionization and that Cu is most likely in a positively charged state. Therefore, enhancement is only driven by consumption of Cui^+ by pair formation with ionized acceptors. As with Fe solubility enhancement, Cu solubility enhancement increases with acceptor concentration as the pairing reaction is driven forward. Also as with the Fe case, Cu solubility enhancement is diminished with increasing temperature due to increased probability for dissociation of the Cu acceptor pair. k is then calculated by taking the ratio of total Cu content in a doped region with the intrinsic Cu solubility. Results are presented in Figures 5 and 6.

Cu Gettering Experiments

We have completed preliminary experiments on Cu gettering in epitaxial p/p+ wafers provided by Komatsu. The epilayers have a resistivity of 11 Ω·cm with substrate resistivity of 5mΩ·cm. Internal Gettering (IG) sites have been intentionally created with a High-Low-High treatment and we have introduced Cu by evaporation at the backside followed by drive in at 950˚C for 20 minutes and an oil quench. FZ Si samples of resistivities 15 Ω·cm and 1100 Ω·cm respectively were subjected to a similar contamination and heat treatment at either 950˚C or 450˚C to saturation followed by an oil quench.

The detection limit of the radiative Cu complex in copper that gives rise to the 1.014 eV no-phonon line is related to doping level due to the formation of the Cu-B pair level which is non-radiative. The radiative Cu related level observed in PL is at E_V + 0.16eV while the non-radiative DLTS level is at E_V + 0.1eV. For Cu concentrations on the order of the doping level, we expect no 1.014eV signal. Extrapolation of known Cu solubility in Si predicts the equilibrium solubility at 950˚C to be $4x10^{17}cm^{-3}$. This value exceeds the doping levels in both FZ materials as well as the epilayers of the epitaxial wafers by 2 orders of magnitude. The solubility limit of Cu in Si at 450˚C for p-type wafers of doping less than $10^{16}cm^{-3}$ is expected to be identical to that of the intrinsic case giving [Cu] = $2x10^{13}cm^{-3}$. Our PL studies demonstrated that the 1.014eV Cu related line could be observed for the case of the 1100 Ω·cm FZ wafer in-diffused at 450˚C and for both the 15 Ω·cm and the 1100 Ω·cm FZ samples in-diffused at 950˚C. The fact that no Cu related line was observed in the epitaxial layer of the epiwafer in-diffused at 950˚C demonstrates qualitatively that Cu is below the detection limit and some amount of gettering from the wafer front surface has occurred.

We performed a step etch on the epitaxial wafers that had been in-diffused at 950°C to reveal different positions in the epilayers as well as layers within the substrate region. PL on all depths within the epilayers revealed no Cu related line. In addition, haze was observed only at depths below the epilayer/substrate interface in contrast to the uniformly doped wafer case where haze is observed near the surface. This provides further evidence for a strong gettering effect of the heavily doped substrate on Cu in the epilayer region during the quench. Since Cu has the ability to homogeneously nucleate without intentionally created IG sites, it is essential to understand the kinetics of the near interface haze in order to accurately simulate Cu gettering. Nevertheless, our current understanding allows us to conclude significant Cu mass transport from the epilayer to the heavily doped substrate must have occurred to make the region of appreciable nucleation and growth of silicide precipitates shift away from the surface to beyond the epilayer/substrate interface. A schematic representation is given in Figure 7.

Gettering Simulator

Our gettering software uses standard solubility relations and diffusion-limited rate equations to create a continuum model for gettering of Fe, Cu, Ni or Co in silicon. The model employs experimentally determined values for diffusivity, ion-pairing binding potentials and precipitate densities. With these parameters, the roles of solubility enhancement, Intrinsic Gettering (IG) precipitation and backside gettering out-diffusion in gettering effectiveness can be evaluated. The variables are p-type doping level, density of bulk IG sites and backside IG site density. We follow the contaminant concentration at arbitrary positions in the wafer as a function of time and temperature. We have developed a user-friendly front end and enabled the simulator to run in a Windows environment.

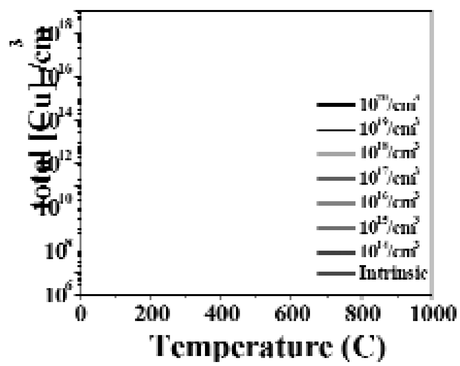

Fig. 5: Total Cu content as a function of temperature is plotted for varying acceptor concentrations.

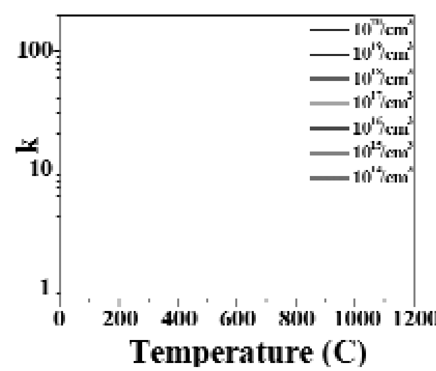

Fig. 6: k is the ratio of Cu Solubility, Cs(Cui), in boron doped Si to that in intrinsic Si. k, the driving force for redistribution from a lightly doped region, increases with increasing boron doping in the heavily doped region or decreasing temperature.

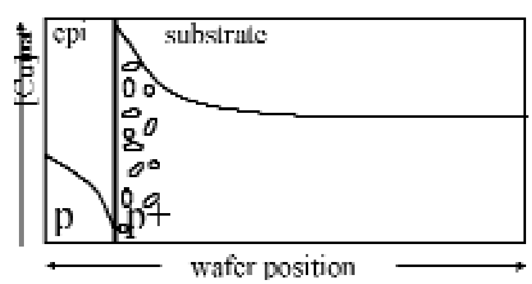

Fig. 7: Schematic of the expected profile of Cu after high temperature in-diffusion followed by a quench. Homogenous silicide formation occurs in the heavily doped substrate near the interface with the epilayer.