Point defect parameter extraction through their reaction with dislocation loops

D. Skarlatos [a], C. Tsamis [a], M. Omri [b] A. Claverie [b] and D. Tsoukalas [a]

[a] Institute of Microelectronics, NCSR 'Demokritos',
15310 Aghia Paraskevi, Greece
[b] CEMES/CNRS, BP 4347,
31055 Cedex Toulouse, France

Abstract

In this work we use dislocation loops to monitor the interstitial injection during the oxidation of silicon at low temperatures (850 – 950 °C). The interstitials captured by the loops are measured using Transmission Electron Microscopy and the number of silicon atoms that are injected into the silicon bulk during oxidation can be estimated. A model is then developed that considers the above measurements and accounts for the silicon supersaturation in the loop layer and subsequently for the flux of injected interstitials during oxidation that is compared with SUPREM IV results. Simulation of loop evolution using FLOOPS simulator permits an estimation of the capturing efficiency of loops in the temperature range of experiments.

1. Introduction and Experiments

A technique proposed by Meng et al. [1] demonstrated that dislocation loops can be used as efficient point defect detectors. This technique offers the advantage of detecting small atom populations and gives the opportunity to quantitatively estimate the number of interstitials injected in Si during a thin oxide formation. In this work we perform a systematic study of the loop distribution in inert and oxidizing ambient in the temperature range 850-950 °C and we compare our experimental results against simulation results using SUPREM IV for the estimation of the number of injected interstitials and FLOOPS for the estimation of the capture efficiency of the dislocation loops.

Our experiments have been launched with Si^+ implantation in Si wafers at 50 keV and dose $2x10^{15}$ cm^{-2} through a thin sacrificial oxide (20 nm). After annealing the wafers at 900 °C for 10 min in N_2 a layer of dislocation loops was formed 110 nm below the surface. Subsequently, the wafers were cut into pairs of companion samples. One of the samples was oxidized in dry O_2 while the other was annealed in N_2 for the same conditions. The thermal treatments were carried out for various temperatures (850°-900°-950 °C) and times (up to 10 h). The imaging of the dislocation loops was performed with Transmission Electron Microscopy. For each sample, at least 500 dislocation loops were measured. The accuracy of the loops measurements is 2 nm. Two

different types of dislocation loops can be identified from the TEM images : a) the circular Frank faulted loops, with smooth edges at the two sides of their long axis and b) the perfect prismatic loops, with more irregular shapes. From the statistical distribution of the loops we can estimate the number of silicon atoms that are bounded in the loops. These experiments are presented in detail in ref. 2.
Another important issue of this work is the determination of the capturing efficiency of a loop layer. Based on a previous set of experiments [2], where the time evolution of two loop layers, separated by less than 2 μm was studied, we estimate that the layer closer to the oxidizing interface absorbs 85% of the injected interstitials. This result will be taken into account later, for the calculation of the number of atoms that are injected into the lattice. This value is in agreement with previous results that estimate the capturing efficiency of the dislocation loops, by studying the Oxidation Enhanced Diffusion of a buried dopant layer and thus monitor the local supersaturation of interstitials below a dislocation loop layer [3,4].

2. Modeling and Simulation results

In the case of oxidation the total number of atoms incorporated in the loop layer is not a constant (as in an inert ambient) but increases with time, since interstitial atoms injected from the silicon surface are constantly incorporated in the loop layer.
For a total loop surface area A cm^{-2} where m loops are present we can write that the change of the number of atoms incorporated within the m loops after interstitial injection by the oxidation process equals the measured change of their number from a TEM picture, N_{net} is the net number of interstitials per unit area in the top loop layer.

$$\sum_{i=1}^{m} \frac{dn_i}{dt} = \frac{d(N_{net}A)}{dt} \qquad (1)$$

Assuming that all the dislocation loops are circular and that the growth of the loops is diffusion limited and can described by the law derived from Hu [5], we find that the average supersaturation of interstitials within the loop layer can be expressed as

$$\frac{\langle C_I^{loop} \rangle}{C_I^*} = \frac{N_{net} \ln(\frac{8\bar{r}}{r_c})}{4\pi^2 \bar{r} d_{loop} D_I C_I^* t} + e^{\frac{\gamma v_m}{bkT}} (1 + \frac{\sigma v_m}{b\bar{r}kT}) \qquad (2)$$

where $\bar{r}$ is the average radius of the loops, d_{loop} equals m/A .
The assumption of a diffusion limited interaction of interstitials with the loops is justified by the results of previous investigations [3,4] as well as by our two loop layer experiments which show that the dislocation loops are efficient sinks for interstitials. Compared with the result obtained by Bonafos et al. [6] for inert ambient, equation (2) contains an additional term which is the first one.
Replacing the numerical values of the parameters involved [5,7] we are able to estimate the interstitial supersaturation within the loop layer as a function of the oxidation time. If we assume no bulk recombination of interstitials with vacancies, the supersaturation of interstitials at the surface during oxidation can be calculated from the equation :

$$D_I C_I^* t \frac{s_I^{surf} - s_I^{loopl}}{a} = N_{Total} \quad (3)$$

Where s_I^{surf} and s_I^{loop1} the average interstitial supersaturation at the surface and at the loop layer, a is he distance of the loop layer from the surface and N_{Total} is the net trapped number of interstitials per unit area taking into account that only 85% of the generated atoms are captured by the loop layer. The results obtained are in good agreement with Packan et al [8].

Figure 1 shows the results we obtain for the total amount of silicon atoms that are injected into the bulk. These data provide a lower limit for the amount of silicon interstitials that must be injected into the silicon lattice during an oxidation process. From these data we can estimate a lower limit for the ratio θ/Ksurf that is used to model interstitials injection during oxidation (parameter θ accounts the generation rate and K_{surf} for the surface recombination rate). These values are listed in table I. Comparison with simulation results shows that the parameters used into simulation tools (SUPREM - FLOOPS) to model interstitial injection, can adequately provide the amount of atoms that are required, if we assume that the existence of the loops does not influence the supersaturation ratio at the surface. However, if the presence of these effective sinks reduces the interstitial supersaturation at the surface, then the number of interstitials that are injected in the bulk without any loop layer could be higher than the calculated above. To answer this problem the recombination velocities at the dislocation loop layer and at the oxidizing interface should be known.

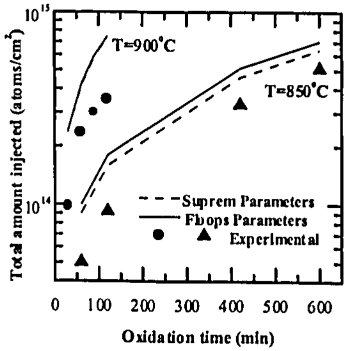

Figure 1. Total amount of silicon atoms injected during silicon oxidation.

Table I. Lower values for θ/k_{surf} ratio.

T (°C)	850	900	950
θ/K_{surf}	345	305	145

The time evolution of the dislocation loops was simulated using the model of Park and Law [9] which is implemented in FLOOPS simulator. However, since this model accounts only for circular loops, we assumed an effective radius for each irregular prismatic loop requiring that the equivalent circular loop has the same area as the one measured by TEM. By this way we create a distribution function that includes both loop populations. This approximation results in a 10% error between the measured by TEM number of bounded atoms and the one given as input value to FLOOPS. The values of the supersaturation of interstitials at the loop layer was estimated from eq (2). As fitting parameters for the simulator we used KI_{loop} (loop-interstitial reaction constant) and a (Capture and emission cross-section).

Figure 2 shows the statistical distribution function of the loop radius after dry oxidation at 850°C. We notice that there is a good agreement with the experimental results,

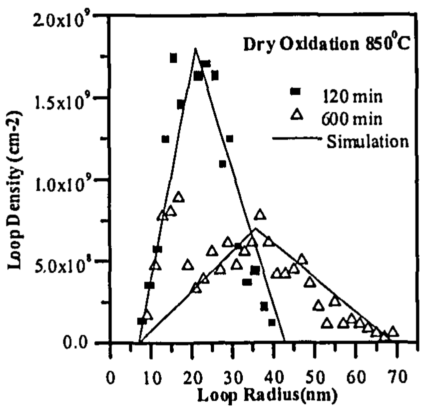

Figure 2. Time evolution of the statistical distribution of dislocation loops.

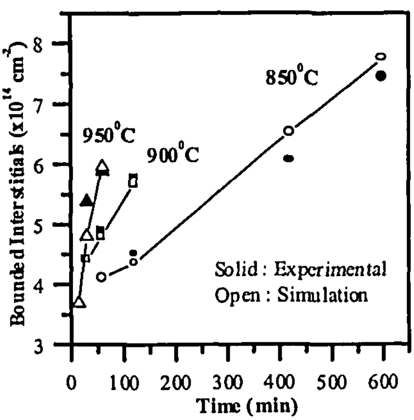

Figure 3. Number of bounded interstitials within the dislocation loops.

although the model implemented in FLOOPS is derived assuming only circular loops, contrary to the experiments. This agreement is probably due to the fact that the relative populations of bounded atoms in both type of loops does not change significantly. The total amount of silicon atoms that are bounded in the dislocation loops as a function of time is shown in fig.3. Again, we observe a good agreement between simulation and experimental results. The extracted value for KI_{loop} is **2.32 10^7 exp(-0.82/kT) sec^{-1}**.

In summary, combining our experimental data with modeling and simulation we estimated interstitial injection parameters in dry oxidation as well as the interstitial capture efficiency of dislocation loops.

This work was supported by EU through the Esprit Long Term Research project "RAPID" (No 23481). We acknowledge Prof. M. Law of the Univ. of Florida and Prof. A. Tasch of the Univ. of Texas for providing FLOOPS code.

References

[1.]H. L. Meng, S. Prussin, M. E. Law and K. S. Jones, J. Appl. Phys., **73**, 955 (1993)

[2.]D. Skarlatos, M. Omri, C. Tsamis, A. Claverie and D. Tsoukalas, Silicon Material Science and Technology Symposium, The Electrochemical Soc., 98-1, p. 914 (1998)

[3.]R. Y. S. Huang and R. W. Dutton, J. Appl. Phys., **74**, 5821 (1993)

[4.]H. Park, H. Robinson, K. S. Jones and M. Law, Appl. Phys. Lett., **65**, 436 (1994)

[5.]S. M Hu, in Defects in Semiconductors, J. Narayan and T. Y. Tan, Editors, p. 333, North-Holland, New York (1981)

[6.] C. Bonafos, M. Omri, B. de Mauduit, G. BenAssayag, A. Claverie, D. Alquier, A. Martinez and D. Mathiot, J. Appl. Phys., **82**, 2855 (1997)

[7.]G. B. Bronner and J. D Plummer, J. Appl. Phys., **61**, 5286 (1987)

[8.]P. A. Packan and J. D. Plummer, J. Appl. Phys., **53**, 6788 (1990)

[9.]H. Park, K. S. Jones and M. E. Law, J. Electrochem. Soc, **141**, 759 (1994)