

## IG Mechanism of Iron in Semiconductor Silicon

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### Introduction

Heavy metals degrade the performance of microchips. Iron is a particularly effective minority carrier lifetime killer [1]. Nevertheless, neither silicon wafers nor devices can be manufactured without processing equipment (e.g. wafering, ion implanting) and consumables (photoresist) that are inexhaustible sources of iron [2]. In order to reduce yield losses due to iron, it ought to be either completely absent in the fab environment and in construction, auxiliary and consumable materials or it must be rendered harmless by means of defect engineering applying internal gettering (IG).

IG is based on tailored precipitation of  $O_i$  yielding  $SiO_{x \leq 2}$  in single crystalline silicon. Varying the initial values of  $O_i$  with a subtle thermal treatment we studied the gettering capacity in B-doped CZ-silicon. We have found a detrimental impact of iron on the  $O_i$ -nucleation and on the growth of these nuclei.

### Experimental

Materials: As-polished, RCA-cleaned ( $Fe < 1.3 \cdot 10^{10}$  at.cm<sup>-2</sup>, silicon wafers (150 mm/diameter, 675  $\mu$ m/thickness, damage-free back side), B-doped (7-22  $\Omega$ cm),  $5.75 \cdot 10^{17}$  at.cm<sup>-3</sup>  $< [O_i] < 8.75 \cdot 10^{17}$  at.cm<sup>-3</sup> CZ [100] and  $[O_i] < 6 \cdot 10^{16}$  at.cm<sup>-3</sup> FZ [100] reference. The wafers were spiked with Fe(Cl<sub>3</sub>) by spin-coating [3] at different stages of thermal treatment:

Sample A: before BMD cycle

Sample B: after Step I

Sample C: after Step II and additional drive-in  
1000°C/6 h/100% O<sub>2</sub>

Thermal treatment, BMD cycle:

Step I 780°C/3 h/100% dry O<sub>2</sub> - nucleation

Step II 1000°C/16h/100% dry O<sub>2</sub> - growth

Analyses: FTIR, EDAX (Mg-K $\alpha$ ) and DLTS (drive-in at (1100°C/10min)

## Results

Fig.1 Fe contamination thwarts precipitation of  $[O_i]$  (sample C).

Fig.2 Varying  $[Fe_i]$  before nucleation (A) we found a critical threshold level of iron (sample A). Below this level the precipitation has occurred as anticipated.

Fig.3 Introducing Fe after the nucleation (sample B, C) did not hinder gettering: IG efficiency > 50%.

Fig.4 EDAX spectrum of a spot (<10 nm, sample A,  $[Fe_i] > 10^{11}$  at.cm<sup>-3</sup>) with  $SiO_x$  nuclei. Fe signal was not detected in every precipitation spots after the BMD cycle.

## Discussion

The formation of thermally unstable  $FeSi_2$  can compete with the nucleation process of  $O_i$ . All the iron cannot be gettered in stable fayalite ( $2FeO.SiO_2$ ) modification because  $FeSi_2$  is stable below 800 °C and it is masking the  $SiO_x$  nuclei. At temperatures around 1000 °C  $FeSi_2$  decomposes and the Fe can be redissolved in silicon (Fig.5). At this temperature the diffusion of Fe is faster than its reaction rate with the  $SiO_x$  particles [4].

The  $Fe_i$  is forming mainly an FeB complex. Both species are effective deep level traps. Generally, an equilibrium manifold has to be considered in order to interpret the influences of heavy metals on nucleation and gettering (Fig.6). The precipitation can be affected through the competitive reaction of interstitials ( $Si_i$ ) with the migrating metal species. The major reaction path is a basic function of the temperature and of the relative concentrations of the active species.

Fig.6 Chemical equilibrium manifold of heavy metals in B-doped silicon (M: heavy metal,  $M_{fac}$ : surface enrichment, k: rate const)

Fig.5 Competitive reaction paths of iron in CZ silicon during gettering

## References

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- [4] B. Hackl, K.-J. Range, H.J. Gores, L. Fabry, P. Stallhofer, J.Electrochem.Soc., 139(11), 3250 (1992)

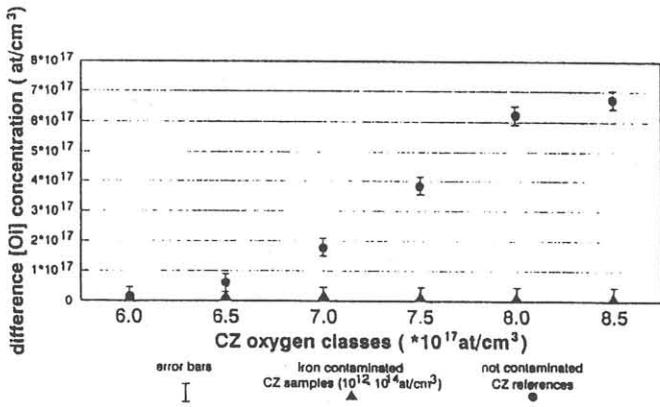


Fig.1 Fe contamination thwarts precipitation of  $[O_i]$  (sample C).

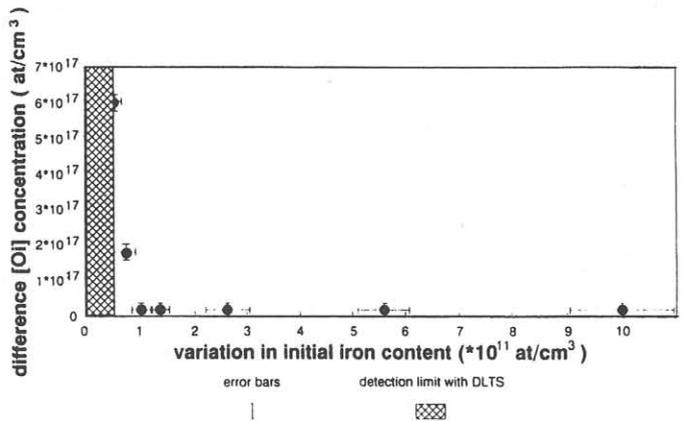
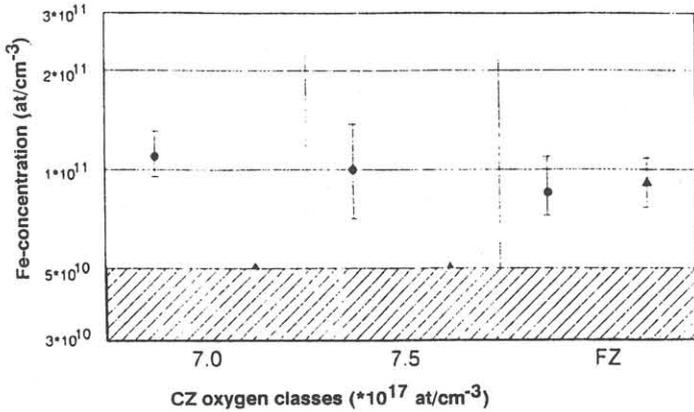


Fig.2 Varying  $[Fe_i]$  before nucleation (A) we found a critical threshold level of iron (sample A). Below this level the precipitation has occurred as anticipated.



● Fe contaminated, w/o BMD cycle    ▲ Fe contaminated sample C    limit of detection    | error bars

Fig.3 Introducing Fe after the nucleation (sample B, C) did not hinder getting: IG efficiency > 50%.

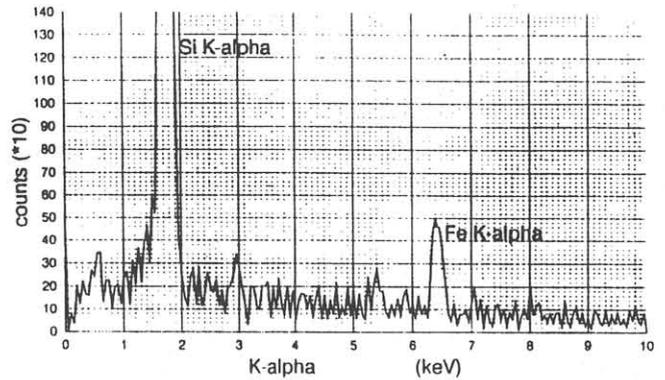


Fig.4 EDAX spectrum of a spot (<10 nm, sample A,  $[Fe_i] > 10^{11}$  at. $cm^{-3}$ ) with  $SiO_x$  nuclei. Fe signal was not detected in every precipitation spots after the BMD cycle.

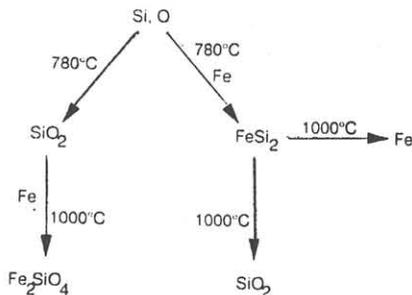


Fig.5 Competitive reaction paths of iron in CZ silicon during getting

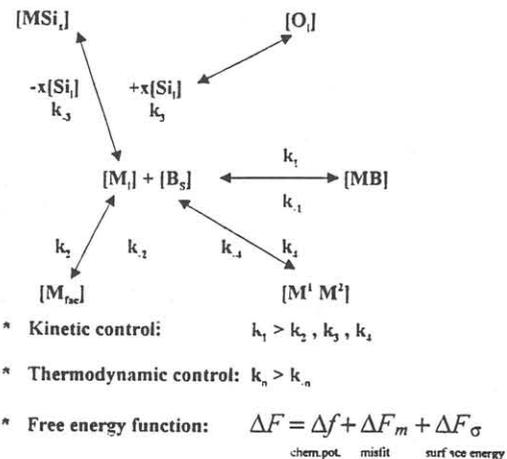


Fig.6 Chemical equilibrium manifold of heavy metals in B-doped silicon (M: heavy metal,  $M_{fac}$ : surface enrichment, k: rate const)