ELECTRON CAPTURE CROSS SECTION OF IRON-BORON PAIRS IN CRYSTALLINE SILICON OVER THE TEMPERATURE RANGE 0 – 100 °C

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ABSTRACT: The electron capture cross section of the acceptor level of iron-boron pairs in crystalline silicon for the temperature range 0 °C to 100 °C has been measured by using a temperature controlled inductive coil lifetime measurement instrument. The characteristic crossover points for which the effective lifetime remains unchanged with the injection density are determined from the plot of injection dependent lifetime curves before and after light soaking of the silicon wafers for different temperatures. The electron capture cross section of iron-boron pairs is then calculated from the slope of the characteristic plot of crossover point density as the function of doping density. The measurements were conducted on four wafers with differing boron concentrations ranging from 1×10^{15} to 5×10^{16} cm^{-3}. Taking published data for the temperature dependence of the capture cross section of interstitial iron in silicon, we find that the electron capture cross section of iron-boron pairs decreases with temperature.
Keywords: Lifetime, Cross over point, Capture cross section.

1. INTRODUCTION

Iron-boron (FeB) pairs form in boron doped silicon in the presence of iron by coulombic attraction between negatively charged substitutional boron (B_s) and positively charged interstitial iron (Fe_i) [1]. Such FeB pairs play a vital role in recombination processes, and exhibit their own unique electronic properties. The coulombic bond between iron and boron can be broken by the external supply of optical, thermal or electrical energy which dissociates the FeB pairs back to isolated Fe_i and B_s atoms. This mechanism of association and dissociation of FeB pairs alters the Fe_i and FeB concentration in the sample. As the defect energy level (ΔE_T), and electron and hole capture cross sections (σ_n, σ_p) of Fe_i and FeB are different, the change in the population of Fe_i and FeB within the silicon wafer alters the lifetime of generated carriers significantly. Despite varying the population of Fe_i and FeB by virtue of association or dissociation processes, the effective lifetime remains unchanged at a particular excess carrier density, which is known as the characteristic crossover point [2]. The characteristic crossover is depicted in fig 1.

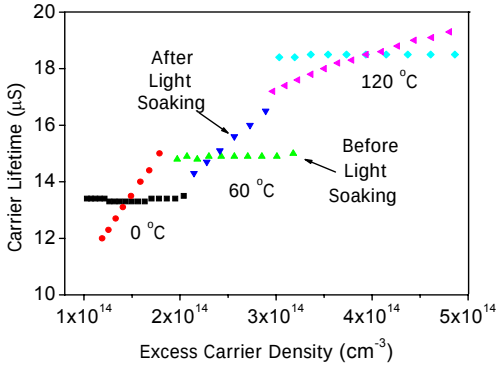

Figure 1: Characteristic crossover point at three different temperatures for Fe-contaminated, B-doped, 1 Ω cm wafer.

At the excess carrier density at which the crossover point occurs (Δn_{COP}), the carrier lifetime due to FeB pairs and Fe_i is the same. This is related to the electron and hole capture cross sections of the FeB pairs in the crystalline silicon. Birkholz *et al.* [3] used the crossover point technique with the doping level to determine the σ_n and σ_p at room temperature, and temperature dependent lifetime data to determine the $\Delta E_{t(FeB)}$, of FeB pairs. This paper describes the application of the crossover point approach used by Brikholz *et al.* [3] for the determination of the $\sigma_{n(FeB)}$, but over the temperature range 0 °C to 100 °C. The temperature dependent lifetime measurement was carried out on a newly developed temperature controlled inductive coil photoconductance (PC) measurement device [4].

2. THEORY

The characteristic crossover point's carrier density (Δn_{COP}) is that for which the carrier lifetime remains unchanged with respect to the degree of dissociation or association of FeB pairs in a silicon wafer. This value is known to be dependent on the doping density and temperature [2, 5]. Hence at crossover points, if we consider solely Shockley-Read-Hall recombination [6, 7] by neglecting the Auger and radiative recombination, then the lifetime at Δn_{COP} can be expressed as;

$$\frac{1}{\tau_{COP}} = \frac{1}{\tau_{associated}} = \frac{1}{\tau_{dissociated}} = \frac{1}{\tau_{SRH,as(FeB)}} + \frac{1}{\tau_{SRH,as(Fei)}} = \frac{1}{\tau_{SRH,dis(FeB)}} + \frac{1}{\tau_{SRH,dis(Fei)}} \quad (1)$$

Where, τ_{as} denotes the associated and τ_{dis} denotes the dissociated lifetime at the crossover point. Birkholz *et al* [3] solved the equation (1) for Δn_{COP} for p-type boron doped silicon with doping concentration, $p_0 \geq 10^{14}$ cm^{-3}, giving:

$$\Delta n_{COP} = \frac{\sigma_n^{-1}(FeB) - \sigma_n^{-1}(Fe_i)}{\sigma_p^{-1}(Fe_i)} p_0 + \frac{\sigma_p(Fe_i)}{\sigma_p(FeB)} N_C \exp\left(-\frac{E_c - E(FeB)}{kT}\right) \quad (2)$$

There are several assumptions made while finding the solution of the third order polynomial in Δn_{COP} derived from the equation (1) and the SRH model [6, 7]. Any trapping effects are neglected, so that the number of excess electrons (Δn) equals the number of excess holes (Δp) in order to simplify the SRH lifetime expression. Two extreme conditions, complete association (FeB only) and complete dissociation (Fe_i only) were assumed in order to simplify the calculation. Furthermore, wafers with doping densities $p_0 \geq 10^{15}$ cm^{-3} were chosen so that the SRH electron and hole densities of interstitial iron ($n_{1(Fei)}$ and $p_{1(Fei)}$), SRH hole

density of FeB pairs ($p_{1(FeB)}$) and equilibrium electron concentration (n_0) can be neglected.
Therefore, from the slope of the linear plot of Δn_{COP} versus doping density (p_0) at different temperatures, and with the values of $\sigma_{n(Fei)}$ and $\sigma_{p(Fei)}$ for each temperature, the temperature dependent values for $\sigma_{n(FeB)}$ can be determined. The trend of the measured $\sigma_{n(FeB)}$ values then can be analysed for evidence of different capture mechanisms, as discussed by Rein [8].

3. EXPERIMENT

The experiment was performed on four boron-doped silicon samples with resistivities 0.6, 1, 4.5 and 13 Ω cm. The average widths of the samples were 250, 490, 199 and 445 microns respectively. Those samples had been intentionally contaminated with iron by ion implantation with an implant dose of 1×10^{11} cm^{-2}. After implantation the samples were annealed at 900 °C for one hour in order to obtain a uniform distribution of iron throughout the bulk. The dose is then divided by the width of the wafer to calculate the Fe concentration within the bulk. In all cases the Fe concentration is below the solubility limit of Fe at 900 °C so that there should be very few Fe atoms in precipitate form. Furthermore each sample was coated with plasma enhanced chemical vapour deposition PECVD silicon nitride in order to ensure that the surface recombination was negligible relative to the bulk recombination.
Lifetime measurements were performed on the newly developed temperature controlled inductive coil PC based device [4] which is suitable for measuring temperature dependent lifetimes for the temperature range -90 °C to 300 °C, however in this experiment the temperature range 0 °C to 100 °C was chosen. The upper limit of the temperature range was chosen as 100 °C, above which $p_{1(Fei)}$ can not be neglected in comparison to the doping density (p_0) in order to satisfy the conditions mentioned in section.2. The experimental setup of the device is depicted in Fig 2. Because of the conductive heating technique applied to heat and cool the wafer, a difference in temperature across the wafer can not be avoided. For these samples, the error in the measured temperature was found to be ± 3% within the wafer, however, in general this is dependent upon the shape and thermal nature of the wafer.

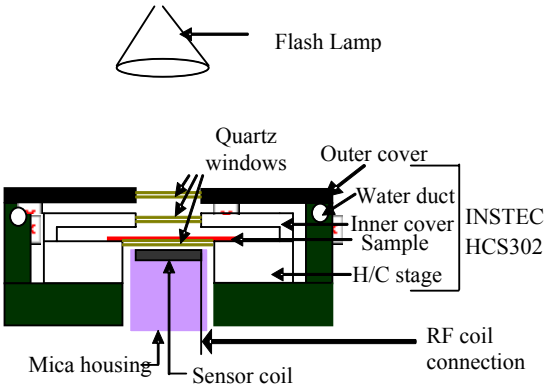

Figure 2: Experimental setup

The lifetime measurement technique is the well established quasi-steady-state photoconductance technique [9]. For this device the error in lifetime measurement was about ± 6%, which was contributed from the wafer thickness (± 2%) and the calibration (± 4%). The error in calibration can be reduced by using test wafers with accurately known doping densities.
Light soaking was used to dissociate the FeB pairs by optical energy. The lifetime was measured before and after the light soaking (2 min) of the sample in order to get the crossover point in lifetime curve as a function of injection density (Δn_{COP}). The experiment was repeated from 0 °C to 100 °C, at 10 °C steps.

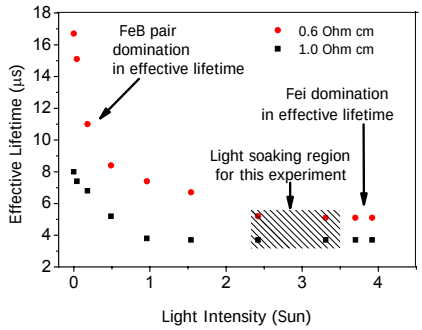

Figure 3: Lifetime with different light soaking intensity for excess carrier density $\Delta n < \Delta n_{COP}$

After pair breaking, effective lifetimes (τ_{eff}) in Fe contaminated p-type silicon become smaller when the excess carrier density (Δn) is lower than Δn_{COP}, and larger when $\Delta n > \Delta n_{COP}$. Conversely, the value of τ_{eff} becomes higher with FeB domination for $\Delta n < \Delta n_{COP}$ and lower for $\Delta n > \Delta n_{COP}$. It is essential to have a sufficient degree of dissociation of the FeB pairs by light soaking to determine the crossover point clearly. An experiment was performed to determine the light intensity and soaking time to ensure the sufficient dissociation of FeB pairs. Figure 3 shows the effective lifetime of 2 samples after 2 min of light soaking at different light intensities. The light intensity chosen for this experiment was ~3 suns, which was sufficient to dissociate significant numbers of FeB pairs in order to clearly identify the crossover point.

4. RESULTS AND DISCUSSION

The injection densities at crossover points were measured at different temperature for each wafer. The change in Δn_{COP} with respect to the temperature for the 1 Ω cm wafer for three different temperatures is depicted in figure 1. Δn_{COP} was found to increase with the temperature, which increases the slope of the linear fit of the plot (Δn_{COP} versus p_0), with respect to temperature, which is shown in fig 4.

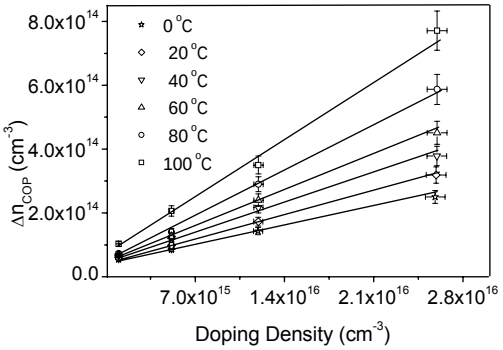

Figure 4: Linear plot of Δn_{COP} versus p_0

In order to calculate the temperature dependent value of the $\sigma_{n(FeB)}$ according to equation 2, we need to supply the temperature dependent value of $\sigma_{n(Fei)}$ and $\sigma_{h(Fei)}$. These values were taken from the literature [10, 11].

$$\sigma_{n(Fei)} = 10^{-10} T^{-1.5} \ [cm^2] \quad (3)$$

$$\sigma_{p(Fei)} = 2.8 \times 10^{-16} \times e^{-0.043 / kT} \ [cm^2] \quad (4)$$

The calculated $\sigma_{n(FeB)}$ on the basis of these literature values of $\sigma_{n(Fei)}$, $\sigma_{p(Fei)}$ and the measured slope for the temperature range is depicted in fig 5. $\sigma_{n(FeB)}$ was found to decrease with the increase in temperature. The error bars for the temperature axis correspond to the temperature difference within the wafer, and the error bars along $\sigma_{n(FeB)}$ corresponds to the total uncertainty in the capture cross section measurement, which includes the error in lifetime measurement, error in locating Δn_{COP} and error in slope measurement (Δn_{COP} versus doping density). The measured value of $\sigma_{n(FeB)}$ in this work near room temperature is found to be comparable with the values measured by Macdonald *et al.* [12] and Rein *et al.*[13], which are also depicted in fig 5. We are unable to compare the measured data for the whole temperature range due to unavailability of previously published data, however the trend is analogous to the temperature dependent value of $\sigma_{n(Fei)}(T)$ as stated in equation 3. The room temperature value published by Birkholz *et al.*[3] is quite different to the measured value in this work. A possible reason for this is that the values of $\sigma_{n(Fei)}$ and $\sigma_{p(Fei)}$ used for the calculations differ. Since the T-dependent value of the $\sigma_{n(FeB)}$ is strongly dependent upon the value $\sigma_{n(Fei)}(T)$, better accuracy of the $\sigma_{n(Fei)}(T)$ data will give more accurate measurement of $\sigma_{n(FeB)}(T)$.

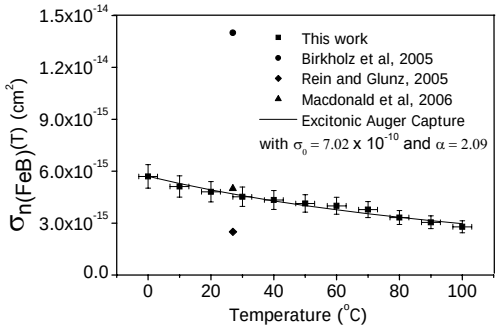

Figure 5: Electron capture cross-section of FeB pairs at different temperature

The best matched T-dependent trends of measured $\sigma_{n(FeB)}$ were expressed in expression (5) and (6) as follows.

$$\sigma_{n(FeB)} = 7.02 \times 10^{-10} T^{-2.09} \quad (5)$$

$$\sigma_{n(FeB)} = 3.35 \times 10^{-14} \exp(-0.00645 \times T) \quad (6)$$

The T-dependent trend of measured values of $\sigma_{n(FeB)}(T)$ was compared with different capture mechanisms [8]. As there is a strong T-dependence in $\sigma_{n(FeB)}$, photon emission capture and classical Auger capture can be ruled out. Furthermore, since the trend is better represented by the negative power of temperature as shown in the expression in (5) than by the exponential function in expression (6), the multi-phonon emission capture (MPE), which can only be represented by a sole exponential function of temperature, seems less likely in this case. In addition, the power of T in expression (5) cannot be -1.4 for our data, which is required for cascade capture due to shallow coulomb attractive centres. Hence this mechanism appears to be ruled out also. Therefore, to explain the trend of measured T-dependent data of $\sigma_{n(FeB)}$, either a two-stage model of cascade capture due to the deep coulomb attractive centres [14] or an excitonic Auger capture mechanism due to the deep centres [15] might be applicable in this case. Fig 5 also shows the plot of excitonic Auger capture with the T-independent capture cross-section pre-factor (σ_0) = 7.02×10^{-10} and the correlation exponent (α) = 2.09 as per equation (5).

5. CONCLUSIONS

The temperature dependent value of the electron capture cross section of FeB pairs in crystalline silicon has been measured using a crossover point technique with a temperature controlled lifetime measurement device. The measured values decrease with the temperature. However, the measured value is strongly dependent upon the literature values of the $\sigma_{n(Fei)}$, and $\sigma_{h(Fei)}$ (equation 2). The uncertainty in the measured values of $\sigma_{n(FeB)}$, could be reduced by using more certain temperature dependent values of the value of $\sigma_{n(Fei)}$, and $\sigma_{h(Fei)}$.

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