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Cross section of the interaction between substitutional B and Si self-interstitials generated by ion beams

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Abstract

The displacement of B from substitutional lattice sites during irradiation with a high energy (650 keV) proton beam is measured by channelling analyses along the ⟨100⟩ and ⟨110⟩ using the $^{11}B(p,\alpha)^{8}Be$ reaction. The normalized B yield, χ, increases with the ion fluence and saturates at a value ($\chi_F < 1$) that depends on the channelling axis, being minimum for channelling along ⟨110⟩. Therefore, displaced B is not randomly located in the lattice. The displacement rate is shown to be consistent with a model involving Si interstitial–B interaction and to depend on the local Si self-interstitial production rate, rather than long range interstitial migration. This was demonstrated by comparing results from samples with and without a Si layer containing 1 at.% C (known to be a trap for interstitial Si) interposed between the B doped layer and the substrate. The B displacement rate does not change in this sample indicating that self-interstitials produced at the end of the range do not play a role in this process. It is therefore concluded that only the Si interstitials produced in the B doped layer contribute to the B displacement and we can fit the damage rate with the following formula: $\chi = \chi_F - [\chi_F - \chi_0]^* \exp(-\sigma^* N_I)$, where χ_0 is the χ of the non-irradiated sample and N_I is the number of (Si interstitials) cm^{-2} calculated by TRIM, with $\sigma \sim 10^{-16}$ cm^2.

Boron–point defect interactions have attracted considerable interest for both fundamental and technological reasons. A lot of works are devoted to the study of the interaction between B atoms and Si self-interstitials, since this interaction affects the B diffusion in the Si matrix and its electrical activation and it determines the formation of electrically inactive B complexes [1–7]. Excellent electrical activation of B in Si based devices is a crucial issue in technological

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development. It is well known that electrically active B atoms are substitutional in the Si lattice and that standard ion beam channelling analysis using the $^{11}B(p,\alpha)^{8}Be$ nuclear reaction at the fixed proton energy of 650 keV [8] is a suitable technique for determining the substitutional fraction of active B atoms. However, it has been reported that B [9] suffers off-lattice displacement during ion beam analysis, and, consequently, electrical de-activation occurs after irradiation at very low fluence, well below the damage threshold of the Si substrate. This has a direct impact on the electronic properties of the material, and a precise and accurate knowledge of the physical mechanism leading to this irradiation induced displacement is required in order to develop reliable devices that operate even under extreme conditions. The interactions of dopants with Si point defects are responsible for several processes including transient enhanced diffusion (TED). As a result, the interaction between point defects and the dopant is well characterized in the high temperature regime, but no data are available for low temperatures. In this work the B displacement during irradiation with a proton beam at room temperature is investigated. In order to obtain the B off-lattice displacement, B doped Si single crystals were irradiated with a proton beam and the B off-lattice displaced fraction measured as a function of the fluence. A proposed model assumes that the B off-lattice displacement process is strictly dependent on the interaction between B substitutional atoms and the Si self-interstitials generated by the incident protons. As a result, the B–I_{Si} trapping cross section at room temperature was evaluated.

A 400 nm thick Si layer uniformly doped with B at a concentration of 1×10^{20} at. cm^{-3} was grown by molecular beam epitaxy (MBE) on an n-type (100) Si substrate. The samples were irradiated at room temperature, using an H^{+} beam with an energy of 650 keV and fluences up to 4×10^{17} H^{+} cm^{-2} at a fixed current of 50 nA. The beam spot was 1 mm^{2}, and it was incident at a random direction on the sample. The proton irradiations were performed using an ultrastable 3.5 MV HVEE Singletron accelerator. Each irradiation was followed by *in situ* NRA channelling measurements along the $\langle 100\rangle$ axis, using the $^{11}B(p,\alpha)^{8}Be$ nuclear reaction at $E_p = 650$ keV. Each channelling analysis was performed using a proton beam fluence of 5×10^{15} H^{+} cm^{-2} to minimize the damage of the sample during analysis. The crystalline quality of the Si lattice was determined simultaneously by detecting the backscattered protons. The detector employed for α particle detection was covered by a 10 μm Mylar foil[2] to prevent a large dead time and the overlapping of the proton and the α signals in the detected α spectrum. The energy integrated α particle yield is proportional to the B concentration seen by the proton incident beam, and the normalized yield, called χ_B, is proportional to the fraction of B displaced from the lattice. NRA channelling analyses on the as-grown sample showed that ~90% of B was substitutional in the lattice. In figure 1 we report the B normalized yield as a function of the irradiating proton fluence. The Si minimum yield is also shown and clearly does not change during the proton irradiation, even at the highest fluence. Therefore the crystalline quality of the Si lattice in the B doped layer remains essentially unchanged during the irradiation. By contrast, the B normalized yield (we refer to sample (a); the experiment on sample (b) will be discussed later) changes drastically after each proton irradiation until it reaches a value of about 0.5 at which it saturates. The χ_B curve starts at an initial χ_B value of $\chi_0 \approx 0.11$ and saturates at a value of $\chi_F \approx 0.57$. Since the measurement of the B normalized yield is proportional to the fraction of B atoms off substitutional sites we can conclude that the proton irradiation induces at room temperature a detectable displacement of B from substitutional positions, while no Si displacement is observed even at the highest proton fluences. The χ_0 value (~0.1) is related to the non-substitutional B fraction in the as-grown sample, while the saturation value (~0.57) indicates that not all of the B atoms are displaced from substitutional

[2] A standard calibration procedure was used to determine the Mylar foil thickness.

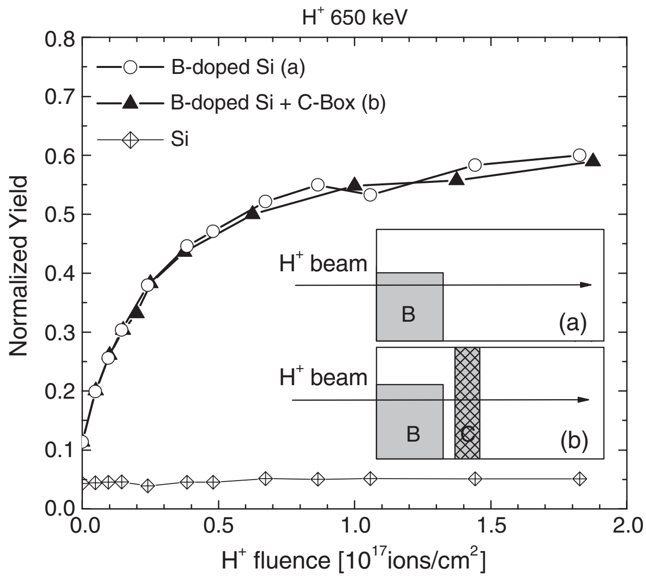

Figure 1. ⟨100⟩ B normalized yields measured by means of NRA as a function of the fluence for proton irradiation at 650 keV for the sample with the Si:C box (▲) and without it (○). The (a) and (b) samples are schematically indicated in the inset.

sites. We prove elsewhere [10] by changing the beam energy that the B displacement is strictly correlated with the energy deposited by the irradiating beam in the doped layer, and that the simplest explanation of this process involves the point defects generated along the ion path and their interaction with substitutional B. A most likely mechanism could be that the off-lattice displacement is mediated by the formation of a mobile B–Si_I couple since it is known that B traps Si_I.

In this experiment the highest Si_I concentration is generated at a depth close to the projected ion range (end of range) (≈8 μm). It is known that I_{Si} can diffuse for several micrometres at room temperature [11], so it is possible that the B off-lattice displacement is due to interactions with Si_I generated along the ion track that reach the B doped region [4–7]. To disentangle the contributions from Si_I generated in the B doped region from that due to Si_I generated along the ion track, measurements were also performed on B doped samples containing a $Si_{1-y}C_y$ alloy box (thickness of 100 nm, $y \sim 0.01$) located 100 nm below the B doped layer (schematically depicted in figure 1 and named sample (b)). It has been demonstrated by several experiments [1] that substitutional C in Si is able to trap Si_I even at RT. We therefore expect variations in the damage rate if Si_I produced deeper in the sample contributes to the displacement. This new sample, with fully substitutional C, was irradiated and analysed in the same manner as the previous one, and the two χ_B curves relative to sample without (a) and with C (b) are plotted against the irradiation fluence in figure 1. Since no difference is observed it is concluded that the B displacement does not depend on Si_I coming from the end-of-range region, but is induced by the interaction with Si_I generated within the B doped layer.

Our data can be interpreted if we model the physical phenomenon on the basis of the following hypothesis: (a) the impurity A binds an interstitial I by forming a mobile couple AI; (b) A migrates in this complex form, AI (the estimated migration barrier is ∼1 eV); (c) the high dopant density (A–A distance ∼2 nm) favours complex formation so the migrating A binds with a substitutional A into a more stable A–A complex; (d) the process ends when there

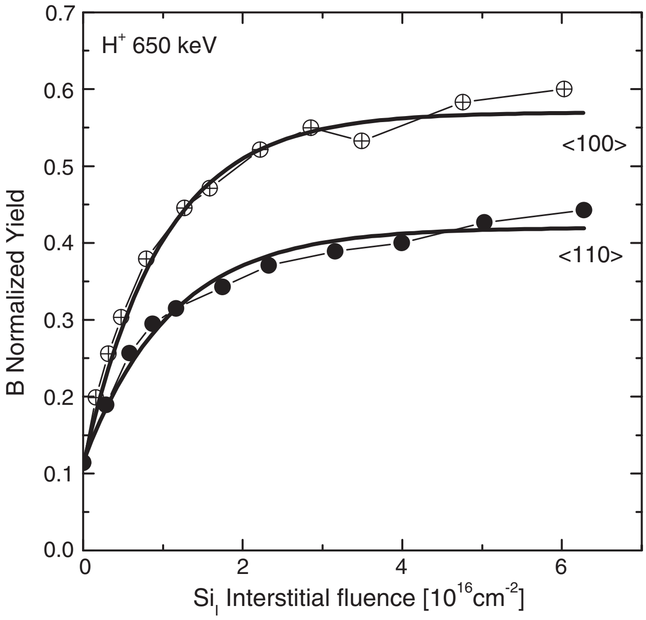

Figure 2. ⟨100⟩ and ⟨110⟩ B normalized yields as a function of the Si–self-interstitial fluence generated by the passing proton beam at 650 keV (⊕). The solid line is the fit of the data using a B–Si_I interaction cross section $\sigma = (1.0 \pm 0.05) \times 10^{-16}$ cm^2.

are no more uncoupled substitutional impurities. If we assume that the limiting step is the Si_I capture process, the variation of the displaced impurity concentration (C_D) can be expressed by

$$\frac{dC_D}{dt} = \sigma_T G_I C_S, \tag{1}$$

where G_I is the rate of the interstitial fluence generated by the impinging beam, C_S is the substitutional impurity concentration and σ_T is the trapping cross section. The C_S at time t can be expressed as

$$C_S(t) = C_{tot} - \gamma C_D, \tag{2}$$

where C_{tot} is the total impurity concentration and γ is a cluster coefficient ($\gamma = 2$ for a cluster formed by two impurity atoms). The solution of equation (2) is

$$C_D(t) = C_{DF} - (C_{DF} - C_{D0}) \exp(-\gamma \sigma_T G_I t); \tag{3}$$

C_{D0} is the initial displaced concentration: in an ideal case it should be zero (it is about 10% of the total concentration in our samples); C_{DF} is the saturation value of the displaced concentration. Since

$$\frac{C_D}{C_T} = f_{\langle hkl\rangle} \chi^{\langle hkl\rangle}, \tag{4}$$

$\chi_{\langle hkl\rangle}$ is the normalized channelling yield along the particular crystallographic axis and $f_{\langle hkl\rangle}$ depends on the ion flux distribution of the particular channel, it is possible to obtain the following expression for χ by substituting equation (4) in (3):

$$\chi(t) = \chi_F - (\chi_F - \chi_0) \exp(-\gamma \sigma_T G_I t) \tag{5}$$

which is equation (1) on setting $\sigma = \gamma\sigma_T$ and $G_I t = N_I$. In this way the fitting parameter σ is the trapping cross section multiplied by the factor γ. The trapping cross section is clearly independent of the particular axial channelling, while σ and the saturation χ_F values depend on the impurity species and cluster configuration. In particular it is known from first-principles calculation that the more stable complex formed at low interstitial injection is a B–B couple [4].

From the above analysis we expect different values of B normalized yield at damage saturation for different channelling orientations, while the B–Si_I interaction cross section σ will be the same since it is not dependent on the axis. In figure 2 we report the curves of the B normalized yield for two different axes ($\langle 100\rangle$ and $\langle 110\rangle$) as a function of the Si_I fluence generated by the proton beam in a 400 nm thick Si layer, calculated by TRIM [12] simulations. From these simulations we obtain the number of Si_I generated by a single ion along its track in that region, a value estimated to be 0.33 I_{Si}/ion for the selected energy of 650 keV. The fit to the data, shown in figure 2 (continuous line), gives $\sigma = (1.0 \pm 0.05) \times 10^{-16}$ cm^2, $\chi_F(\langle 100\rangle) = 0.57$ and $\chi_F(\langle 110\rangle) = 0.42$. On the basis of this result, it is concluded that the B_S atom has a capture radius for the generated I_{Si} of about 0.06 nm.

In conclusion, the displacement of B atoms out of crystalline sites induced at RT by proton irradiations has been investigated. The measured displaced B fraction increases with the total fluence of the irradiation until it reaches a saturation value lower than unity. Experimental data have been fitted assuming an interaction between the excess of Si_I generated by the beam and the substitutional B atoms, and the B–Si_I trapping cross section at room temperature has been evaluated.

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