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Optical and electrical activity of boron interstitial defects in Si

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Abstract

Density functional theory is used to investigate boron interstitial clusters and defects formed with carbon and oxygen. Using data from experimental techniques such as deep level transient spectroscopy, and electron paramagnetic resonance, photoluminescence and infrared studies, we are able to assign structures to many observed centres and begin to develop a series of reaction paths for the evolution of boron with annealing temperature depending on the relative concentrations of impurities.

Among other results we demonstrate that a metastable defect composed of two boron interstitials and a self-interstitial has symmetry, vibrational modes and an electronic structure consistent with the I2 photoluminescence centre, also known as the Y centre.

1. Introduction

Understanding the reaction paths of ion implanted B in Si is of great importance to the semiconductor device industry. Indeed, a detailed understanding of these processes is essential to the development of accurate front end simulations for Si device designers and manufactures. Semiconductor devices consist of shallow and abrupt regions with dopant concentrations at levels well above their solid solubility limit. Currently the best available means for achieving such an arrangement is to ion implant the dopant into the specific regions of the semiconductor where the highly doped regions are required. This must be followed by an anneal to activate the dopant and to repair some of the lattice damage (Frenkel pairs, for example) caused by the implanted ions. In the case of B implanted into Si it is at this stage where the undesirable and widely studied phenomenon of transient enhanced diffusion (TED) is observed. For a recent review of TED see [1]. It is believed that as the sample is annealed {113} defects present in the Si undergo Ostwald ripening and a wind of self-interstitials is created as they

diffuse from smaller {113} clusters to larger {113} clusters. These larger {113} clusters grow at the expense of the smaller ones [2, 3]. As this wind of self-interstitials blows through the heavily B doped region some of them will be trapped by B_s and since boron is known to diffuse via self-interstitials a large diffusion of boron will occur. The consequences of this are, first, that the abrupt division between the doped and undoped regions becomes smeared and, second, much of the boron in the most highly doped regions forms clusters with the self-interstitials. Some of these immobile clusters are highly stable and since their formation prevents the B assuming a substitutional position they lead to an undesirable reduction in the electrical activity of the dopant [4]. Hence it is important to study the properties of these boron interstitial clusters (BICs) so that we may better understand the mechanisms leading to their formation and perhaps find ways to prevent their formation.

It is not just self-interstitials that interact and complex with the implanted B. Even in relatively pure Si many impurities are still found. Typically a significant concentration of oxygen and carbon will be present and the interaction of these impurities with B can also lead to clusters of varying electrical activity.

In order to study these complexes low energy structures are found with properties in agreement with those of experimentally observed centres. Infrared (IR) absorption experiments have been performed on electron irradiated, B doped Si that has been compensated by co-doping with either P or As [5]. It is found that electron irradiating the sample at low temperature produces self-interstitials which may be trapped by B_s forming B_i. This gives rise to the LVMs labelled the R lines. The Si-G28 EPR centre has also been assigned to B_i [6] and later EPR and DLTS experiments [7] showed B_i to be a negative-U defect with C_{1h} symmetry in the negative and neutral charge states and C_{3v} in the positive. The donor level was found to be at $E_{\rm c} - 0.13$ eV with the acceptor level at $E_{\rm c} - 0.37$ eV. Isothermal anneals reveal that the defect responsible for the R lines anneals at around 230 K and a new set of modes are observed, labelled the S lines [5]. The defect responsible for these modes only exists over a narrow temperature range (\sim 225 to just above 300 K) and is converted into a defect giving rise to a set of LVMs labelled the Q lines. The defect giving rise to these Q lines is stable to above 300 K and separate experiments find that it anneals at ~220 °C [8]. A set of modes labelled the P lines and assigned to a substitutional B pair are present throughout the anneals. This grown in defect is stable above 300 K [5].

At temperatures greater than 300 K free carriers prevent further IR experiments and so alternative techniques must be employed to study more stable clusters. A photoluminescence (PL) centre is formed in B implanted or electron irradiated Si which has been annealed to around 350 °C with a zero phonon line at 1.080 eV [9]. This is known as either the I2 or Y line. The I2 line consists of four 'peaks' and by implanting different isotopes of B it was shown that the I2 defect consists of two optically equivalent B atoms. The centre is found to have a local mode satellite shifted from the zero phonon line by -30.2 meV (labelled L1) and later a second local mode satellite (labelled L2) was observed, shifted from the zero phonon line by 104.6 meV (¹¹B) and 109.4 meV (¹⁰B) [10]. These modes again display the same isotope effects. L1 is reported to display a small isotope effect (¹⁰B: 30.18 meV and ¹¹B: 30.04 meV). These modes are given in units of wavenumbers in table 2, discussed below. It is noted in this later work that a slight shift between the deconvoluted positions of the modes from the fourfold structure for the natural isotopic abundances of B and those observed in the isotopically pure cases implies that the two B are only very nearly equivalent. Zeeman measurements indicate trigonal symmetry although uniaxial stress measurements reveal the true symmetry to be C_{1h}.

Several DLTS studies have revealed levels formed by complexes of boron and common impurities. In B doped Si electron irradiated at cryogenic temperatures B_i is formed in equal concentration to V through the reaction $B_s + Si_i \rightarrow B_i$. The disappearance of the single

Table 1. The calculated and observed electrical levels of BICs and boron–impurity complexes in Si along with their observed annealing temperatures. The positions of levels are given with respect to the valence band top assuming a Si band gap of 1.2 where a conversion was necessary.

	<i>E</i> (-/0) (eV)	<i>E</i> (0/+) (eV)	Annealing temperature (K)
Bs	0.2 (0.05 [18])	None	>300 [5]
B_2	0.17	None	>300 [5]
BI	0.87 (0.83 [7])	0.87 (1.07 [7])	230 [5]
B_2I^S	1.00	None	270 [5]
B_2I^Q	None	None	500 [8]
$B_2I_3^Y$	~ 1.0	~ 0.2	
BiOi	None	0.98 (~0.97 [11-13])	~420 [11–13]
B_iC_s	~ 0.9	~0.2 (~0.3 [12, 13])	675 [12, 13]

acceptor level of B_i is correlated with the growth of a level at $E_c - 0.23$ eV at ~240 K. This level is observed in both p- and n-type Si [11]. Alternatively, electron irradiation at room temperature also introduces a large number of boron interstitials. B_i which is mobile at room temperature [6] will then be trapped by other impurities such as carbon or oxygen. The first boron related level to form is reported at $E_c - 0.27 \text{ eV}$ [12] and is believed to be the same as the level reported at $E_{\rm c} - 0.23$ eV. The $E_{\rm c} - 0.27$ eV level has a production rate proportional to $[B]^{1/2}$ and a capture cross section of 3×10^{-13} cm² implying a single (0/+) or double (+/2+) donor level [12]. This level anneals at 170 °C giving rise to a new level at E_v + 0.30 eV with a frequency factor for formation of $\nu = 1.5 \times 10^{11} \text{ s}^{-1}$ and activation energy $E_{\rm A} = 1.2 \text{ eV}$, the same frequency factor and activation energy as observed for the decay of the $E_c - 0.27$ eV level. Hence there is strong evidence that this $E_v + 0.30$ eV level is caused by a defect that has evolved from the defect giving rise to the $E_c - 0.27$ eV level. The $E_v + 0.30$ eV level anneals at 400 °C. Similar levels have been found by another study into room temperature electron irradiated Si [13]. This time a level is found at $E_c - 0.26 \text{ eV}$ (again we believe this is the same as that reported at $E_{\rm c} - 0.23$ eV) with a production rate proportional to [B]¹ but in highly B doped material the production rate decays as $[B]^{-2}$ probably due to the formation of $B_2 I^Q$ ($B_s B_i$), discussed below. The production rate is also proportional to [O] strongly suggesting that the defect causing the level is B_iO_i . The $E_c - 0.26$ eV level anneals by dissociation at around 150 °C (depending on [O]) giving rise to a level at $E_v + 0.29$ eV which we believe is the same level as that reported to be at $E_v + 0.30$ eV. The production rate of this $E_v + 0.29$ eV level is inversely proportional to [B] and is independent of [O] but directly proportional to [C]. This leads to the assumption that the $E_v + 0.29$ eV level is due to B_iC_s which is formed as B_iO_i dissociates and B_i is trapped by C_s.

2. Method

The spin-polarized density functional theory (DFT) code AIMPRO was used to investigate possible B complexes that may give rise to these levels. The code uses Gaussian basis sets. Bachelet–Hamann–Schlüter pseudopotentials [14] are used for Si, O and C and a Troullier–Martins pseudopotential [15] is used for B. A Monkhorst–Pack $2 \times 2 \times 2$ sampling scheme was used for all defect supercells [16]. Supercells of 64 atoms were typically used although for some of the larger defects (B₂I₃^Y, for example) 216 supercells were required. A discussion of the method and convergence tests has been given elsewhere [17] and will not be repeated here.



Figure 1. The structures of B clusters studied in this paper with a section of bulk Si (a) to aid the reader. Dark atoms represent B and small white atoms are Si interstitials. (b) $(B_s-Si_i) (C_{3\nu})$ and (c) $B_i^X (C_{1h})$, the two charge dependent structures of BI. (d) B_2I^S and (e) B_2I^Q , the metastable and stable forms of B_2I . (f) I_3^W , the I1 or W centre. (g) The $B_2I_3^Y$ defect and (h) lower energy $B_2I_3^{fr}$ as found in [19].

3. Results

3.1. Boron interstitial clusters

In this section only a brief summary of our results will be given as they have been reported in greater detail elsewhere [17]. A summary of calculated and measured LVMs and electrical levels is given in table 2 and the corresponding defect structures are shown in figure 1. A summary of annealing temperatures and electrical levels is given in table 1. To describe different BICs we have adopted the notation of the Motorola group as used in, for example, [19]. A BIC is referred to as $B_n I_m$ where n is the number of B atoms and m is the total number of interstitial atoms of either species. The structure we find for BI is the same as reported in [20–23], our calculated LVMs providing firm confirmation that this is indeed the correct structure. The modes assigned to $B(B_s)$ and B_2 (the P lines) agree very well. It is interesting to note that B_2 (the B_s-B_s pair) is actually a metastable defect whose formation energy decreases as a function of separation until the formation energy of B_s is asymptotically reached. This is in agreement with the work of [19, 21, 24, 25] and is evidence for the existence of defects which are clearly metastable. Furthermore the isomer of B_2I that we have called B_2I^S , the defect we assign to the S lines, is actually a metastable form of B_2I^Q , the defect we assign to the Q lines in agreement with [24]. This sits comfortably in the model where B_i anneals and becomes mobile at \sim 240 K, diffuses to another B_i and forms the Q centre, B₂I^Q, via its metastable form B₂I^S. Turning to the PL centre [9, 10] it is again a metastable defect that is found to have properties in agreement with the I2 lines. The $B_2I_3^Y$ defect that we assign to the I2 centre is a metastable defect. The stable form in agreement with [19] is shown in figure 1 labelled $B_2I_3^{6r}$. $B_2I_3^{6r}$ can be ruled out as a candidate for being the I2 centre since it has an electrical level close to mid-gap. Furthermore it does not possess the C1h symmetry of the I2 centre. Why this defect is not observed experimentally is unclear but possibly, due to the complicated nature of its structure, it is never able to form. The $B_2I_3^Y$ defect on the other hand is very similar to the structure of the I1 centre [26, 27].



Figure 2. (a) A sample of bulk Si; (b) the B_iO_i defect; (c) the B_iC_s defect. Si atoms are shown in grey, the B are represented by small black balls, the C are represented by the larger white balls while the small white ball represents O.

Table 2. The experimental and calculated local vibrational modes (cm^{-1}) of B_s , BI, B_sB_s , the two B_2I defects (assigned to the S and Q centres) and $B_2I_3^Y$ and their corresponding isotopic shifts. The experimental values are given in parentheses. All modes are taken from [5] with the exception of those belonging to the I2 centre which are taken from [10].

				Mixed isotope
	¹¹ B	¹⁰ B	Shift	mode
B-				
T ₂	626 (¹¹ B _s 623)	650 (¹⁰ B _s 646)	24 (23)	NA
$BI^+(C_{3v})$				
A ₁	697 (¹¹ R 730)	726 (¹⁰ R 757)	29 (27)	NA
B_{2}^{2-}				
A _{1g}	635	664	29	650
Eg	602	627	25	617
Eu	551 (P ₁ 553)	568 (P3 570)	17 (17)	558 (P2 560)
$B_2 I^S$				
A_{2u}	919 (S ₁ 903)	946 (S ₃ 928)	27 (25)	934 (S ₂ 917)
A _{1g}	702	736	34	718
Eu	611 (S ₄ 599)	634	23	628 (S ₅ 603)
Eg	595	616	21	600
B_2I^Q				
A ₁	1132	1186	54	1159
E	756 (¹¹ Q 733)	785 (¹⁰ Q 760)	29 (27)	785, 756
$B_2I_3^Y$				
A'	1043	1093	50	1068
Α″	808	841	33	836
A'	801 (I2 843)	832 (I2 882)	31 (39)	804
Α″	580	591	11	584
A′	578	581	2	580
A′	563	567	5	565
A′	552	556	3	554
Α″	232 (I2 242)	234 (I2 242)	2 (<1)	233

3.2. Boron-impurity complexes

The lowest energy structure of B_iO_i is found to be that shown in figure 2. This can be thought of as a $\langle 100 \rangle$ boron split interstitial next to a puckered bond centred interstitial oxygen. This structure is clearly similar to that found for C_iO_i [28, 29]. We find that B_i is bound to O_i by 0.6 eV (E_B). Given that the migration energy (W) of B_i is 0.6 eV [11] an activation energy for dissociation of $W + E_B = 1.2$ eV is found. This is in superb agreement with the value deduced through isothermal anneals of $E_A = 1.2 \pm 0.1$ eV [12]. We find that this defect has a single donor level at around $E_c - 0.22$ eV in very good agreement with that observed around $E_c - 0.23$ eV. We calculate a double donor level to lie extremely low in the gap at $\sim E_v + 0.06$ eV and so we show that the level at $\sim E_c - 0.23$ eV must actually be a single donor (0/+) rather than double donor (+/2+) level, contrary to the majority carrier caption cross section analysis [12]. Clearly this provides firm evidence that the $\sim E_c - 0.23$ eV level is indeed due to B_iO_i which has the structure shown in figure 2.

For B_iC_s we find the most stable configuration to be very similar to B_2I^Q (or B_sB_i), the $\langle 100 \rangle$ boron split interstitial which is known to be highly stable. B_iC_s is a similar structure with one boron atom replaced by a carbon atom (figure 2). This is in agreement with previous work [30]. As may be expected, since the carbon atom is undercoordinated it may easily donate an electron. We place the donor level at around $E_v + 0.2$ eV using a 216 atom supercell. This is in agreement with the level observed around $E_v + 0.30$ eV. We also predict that the defect has a single acceptor level in the upper part of the band gap. Before we consider the thermal stability of this defect we must first consider how it will dissociate. We calculate that a self-interstitial is more tightly bound to C_s than B_s by around 0.7 eV. The binding energy of C_i to B_s is found to be 1.2 eV (E_B) and the migration energy (W) measured to be 0.88 eV [31], so assuming $\nu \approx 10^{13} \text{ s}^{-1}$ an estimate of the temperature that the defect will dissociate at can be calculated as $T = (W + E_B)/k \ln \nu$. The temperature that we estimate is ~400 °C, in agreement with the measured annealing temperature.

4. Discussion and conclusions

We have now provided evidence from *ab initio* calculations which in conjunction with observed electrical levels or IR absorption assigns defect structures to many BICs and two of the most important boron–impurity complexes known to form in Si. From this we may then develop a model for the evolution of B in Si with temperature through the evolution and formation of clusters of higher and higher stability.

If we consider electron irradiated, B doped Si, it is known that the radiation will produce self-interstitials which will very efficiently be trapped by B_s creating BI (B_i) with its corresponding IR absorption lines (the R lines) and electrical levels. Alternatively if B is introduced by ion implantation a large fraction of it will already be interstitial (~70% [32] depending on implantation conditions). The remaining substitutional B is very stable and will remain in the Si as indeed does the substitutional B pair, the defect that gives rise to the P lines. BI will anneal at 230 K when it becomes mobile and diffuses to a second BI forming the B_2I^Q defect (the B_sB_i (100) split interstitial) via its metastable isomer B_2I^S . This highly stable, electrically inactive defect will not anneal until around 220 °C. We have shown previously that this is not due to dissociation but rather due to a reaction with V₂ which becomes mobile around this temperature, in accordance with [8]. In regions where there is an abundance of self-interstitials it is possible that B_2I^Q will instead react with a mobile di-interstitial forming the metastable $B_2I_3^Q$ defect, the defect most probably responsible for the I2 lines. This will not anneal until around 400 °C [33] or 500 °C [34]. It is around this temperature that there has been shown to be a large recovery in the substitutional fraction of B [35].

Alternative reaction paths (when the impurity content is high or B content low) involve common impurities that are present in Si, namely oxygen and carbon. We have shown here that an alternative defect that can be formed from the annealing of B_i is B_iO_i. This defect gives rise to an electrical level at around $E_c - 0.23$ eV and is stable until ~150 °C when it anneals by dissociation. The formation of B_iC_s then follows giving rise to a single donor level at ~ $E_v + 0.30$ eV. This defect may be created by the B_i reacting with C_iC_s with the release of C_i although this is speculation and further investigation is required. This B_iC_s defect is then stable until around 400 °C. Again we note that around this temperature a large recovery in the substitutional fraction of B takes place.

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