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Passivation of boron in silicon by hydrogen and muonium: calculation of electric field gradients, quadrupole resonance frequencies and cross relaxation functions

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Abstract. The possibility of studying impurity passivation complexes in semiconductors by quadrupole resonance spectroscopy is examined. The problem is illustrated for the case of boron in silicon passivated with hydrogen or, equivalently, with muonium, since the radioactive light isotope in principle offers a greater sensitivity for detection of the spectra. *Ab initio* calculations on suitable cluster models of the passivation complexes provide estimates of the electric field gradients at the quadrupolar nuclei, and thereby predictions of the quadrupole resonance frequencies. Detection via cross-relaxation techniques is proposed, notably muon level crossing resonance (μLCR), and illustrated by calculation of the time dependence of the muon polarization function. Possible reasons for the absence of quadrupolar resonances in μLCR spectra recorded in exploratory experiments are discussed; these include the existence of a local tunnelling mode for the lighter isotope.

1. Introduction

The passivation of both donor and acceptor impurities in semiconductors by hydrogen is currently attracting considerable interest [1]. The complexes have been detected experimentally by infrared (IR) and Raman spectroscopy and a number of theoretical studies of their quantum electronic structure have been published. Generally, three different sites of the hydrogen relative to the impurity are discussed, namely bond-centred, antibonding to the defect or antibonding to an adjacent host atom.

Additional microscopic and structural information on the complexes, e.g. of the type offered by one of the nuclear probe spectroscopies, would evidently be valuable. The normally low concentration in which the complexes are present sides against success with conventional magnetic resonance, although experiments on highly doped samples are worth considering. In this paper we calculate the quadrupole resonance frequencies which would provide signatures of the various configurations. We also aim to demonstrate that the technique of muon level crossing resonance (μLCR) should be applicable. In this extremely sensitive technique, implanted positive muons mimic the behaviour of the proton and detailed spectroscopic information is available

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when the muons adopt a lattice position adjacent to a quadrupolar nucleus; the technique is closely analogous to quadrupole cross relaxation spectroscopy [2]. It is well known that muons stopped in pure group IV semiconductors form two paramagnetic states of interstitial muonium [3]. One of these, denoted (Mu'), is isotropic and corresponds to the hydrogen-like atom diffusing rapidly between tetrahedral cages. The other, denoted Mu*, has trigonal symmetry and its bond-centre location [4] is verified both by experimental and theoretical studies [5]. Although analogous states should in principle exist for isolated interstitial hydrogen atoms, hydrogen is in fact detectable in semiconductors only in association with other impurities [6,7], except for a single ESR observation [8]. The proposal to study diamagnetic muonium–impurity complexes by level crossing resonance, made recently by one of us [7,9], is examined in detail here for the case of silicon doped with boron. Similar considerations should apply to complexes with other acceptors having quadrupolar nuclei, e.g. gallium and aluminium.

Since the recognition that hydrogen can pair with a boron impurity in silicon [10], removing their individual electrically active levels from the energy gap, this is the example of passivation which has received greatest attention in the literature. The preferred location of the proton close to a B–Si bond-centre (known also as the bondminimum) appears now to be largely substantiated. This is found to be the minimum energy configuration by authors using various computational methods, e.g. *ab initio* (Hartree–Fock) [11–13], local density functional [14] and semi-empirical (MNDO) [15,16]. Experimentally the sharp IR line at 1880 cm^{-1} [17], exhibiting the expected isotope shifts on deuteration, as well as Raman spectra [18,19] are taken to be fully supportive of this model. There is some discussion as to whether the global minimum of energy is exactly in line with the boron and silicon nuclei or whether the trigonal symmetry is broken: some authors find the minimum to be displaced laterally from the bond-centre [12,20]. On this point the experimental data is inconclusive [18,21–23].

For a given boron impurity, taken to be substitutional in the silicon lattice, there are four bond-centred sites adjacent, which are equivalent in the absence of local strain. The possibility of thermally activated hopping of protons between them has been demonstrated [17] with the conclusion that the activation energy involved is as little as 0.19 eV. Subsidiary local minima exist at the antibonding sites adjacent to both the nearest-neighbour silicon atoms [11,12,13,20] and to the boron itself [13,24]. Some authors find the boron antibonding site to correspond to a saddle point only, however, in [12,14,16,25], by the use of valence force analysis, its occupation was found to be incompatible with the available data. The silicon antibonding site is the deeper of the two and there is some evidence of its partial occupation from channelling data [22]. It is noteworthy that the silicon antibonding site is favoured in the passivation of donors, e.g. phosphorus [26].

Since the same adiabatic energy surface is held to govern the behaviour of both muons and protons, these particles should have the same equilibrium positions. That is, implanted muons should also trap close to boron impurities in silicon; either as a result of an encounter with the rapidly diffusing Mu' fraction, or through the more direct effect of the boron defects on the thermalization process.

The objective of the present study is the detection of boron–muonium or boron–hydrogen complexes via cross relaxation between the muons or protons and the boron nuclei. The muon experiment is an application of μLCR to a diamagnetic or closed-shell system in the form proposed by Abragam [2] in which the muon spin is put

on speaking terms with a neighbouring nuclear spin by tuning an applied magnetic field so that the muon Zeeman energy just matches the nuclear quadrupole splitting. A resonant loss of muon polarization due to flip–flop transitions is then detected via the asymmetry in the muon decay. Such resonances have been demonstrated for interstitial muons in metallic copper [27], for muons adjacent to ^{17}O nuclei in several systems [28,29], and most recently for muons interacting with ^{55}Mn nuclei in MnSi [30]. Both the position and the strength of the resonances are informative on details of the local structure, and so can be used to confront the theoretical model. In the present instance, the theoretical model in question is a simulation of the quantum electronic structure of the passivation complexes by *ab initio* methods, along the lines of those reported previously [11,12] but extended in the present work to include calculations of the electric field gradients at the nuclei concerned; these calculations are described in section 2. From these gradients, the quadrupole resonance frequencies are readily predicted; simulation of the resonances involves evaluation of the appropriate cross relaxation functions, which is illustrated for the muon case in section 3.

With a mass ratio of $m_\mu/m_p = 1/9$, the muon is not so light as to invalidate the adiabatic approximation but its dynamical behaviour may be expected to differ significantly from that of the proton. Occupation of the various sites has to be reconsidered for the muon case, both by virtue of the greater spread of its wavefunction (larger zero-point energy) and the possible population of metastable states on the microsecond time scale of the muon implantation experiments. These points are considered in section 4, together with the likelihood of coherent tunnelling of the lighter particle.

2. Cluster calculations

We have therefore calculated the lowest energy configuration of the (B,H) complex in silicon with B substituting a host atom and H (Mu) in a nearby bond-centre using *ab initio* all-electron cluster calculations at the restricted Hartree–Fock level. To this end the Si–Si bond length R_{Si-Si} and the bondlength R_{Si-H} of the saturating H atoms have been optimized in a Si_8H_{18} cluster. Using the split-valence 3–21 g basis-set (single-zeta quality for the core electrons and double-zeta for the valence ones) the values $R_{Si-Si} = 2.38$ Å and $R_{Si-H} = 1.49$ Å were obtained, which compare well with the experimental value of $R_{Si-Si} = 2.351$ Å and theoretical investigations on similar clusters [12]. Next, a silicon atom was replaced by a boron and an additional hydrogen atom was placed along the bond axis. The coordinates of the three neighbouring atoms B, H, and Si were then optimized enforcing C_{3v} symmetry. In the final calculations the expanded basis-sets on boron, hydrogen and adjacent silicon atom were used (split-valence basis sets 6–31 g with additional *d* functions on B and Si and *p* function on H). The resulting equilibrium structure is shown in figure 1.

The elements of the electric field gradient tensor were then calculated from the wavefunction describing this equilibrium structure. The results obtained, including the values for the two metastable configurations, are presented in table 1. Strictly, these values correspond to the proton (or muon) held static at the respective sites. We assume, as a first approximation, that the dynamic averages over the zero-point motion of the muon are not substantially different from these values. For the bond-centre site, for instance, a displacement of H (Mu) from its equilibrium position by

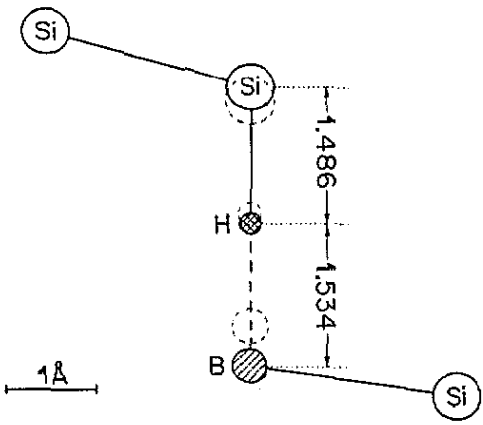

Figure 1. Calculated geometry of the lowest energy configuration of the (B,H) complex in silicon. The distances are given in Å, and the dashed circles indicate the location of the undisturbed substitutional sites.

Table 1. Calculated H–B distance d in Å and the elements of the electric field gradient tensor V_{xx}, V_{yy} and V_{zz} (in principal axes) experienced by the B nucleus (in atomic units; 1 au = 0.972 V cm^2). The results are presented for the lowest energy configuration (BC), where H is placed at the bond-minimum site, as well as for the two antibonding configurations (to one of the 4 adjacent Si atoms (AB to Si) and to B itself (AB to B)).

Site	d	$V_{xx} = V_{yy}$	V_{zz}
BC	1.499	0.188	−0.376
AB to Si	5.015	0.213	−0.426
AB to B	1.208	−0.036	0.072

0.1 Å results in a change of V_{zz} of about 10%, and for the two possible directions along the B–Si bond these changes are of opposite signs†.

As a guide to the accuracy of these predictions, we note that test calculations by the same methods on simple molecules such as H_2 ^{17}O and $Si^{35}Cl_4$ give values for the electric field gradients which agree with experimental results in the NQR literature to better than 10%. A description of these tests on model systems, showing how the predictions converge as the basis set is enlarged, will be given elsewhere. It is worth mentioning here that greater accuracy is expected for quantities relating to *charge density* in closed shell systems than for *spin density* in open shell systems (the latter requiring unrestricted Hartree–Fock wavefunctions, with their inherent errors for the estimation of hyperfine couplings, or else more sophisticated post Hartree–Fock methods). For the present purpose of estimating quadrupole couplings, the use of all-electron calculations rather than pseudo-potential methods eliminates uncertainty concerning Sternheimer screening of the potentials at the nuclei. Conversion from electric field gradients to quadrupole frequencies may in fact be the greatest source of error, the accuracy with which the nuclear quadrupole moments are known being the limiting factor in many cases. Simulation of the μLCR spectra, given the nuclear positions and appropriate electric field gradients, is the subject of the following section.

† In fact, the different dynamic averages for muon and proton should give rise to a small but significant difference in the boron quadrupole coupling constants between muonium–boron and hydrogen–boron complexes. Such an isotope effect has already been observed for the case of muons and protons adjacent to ^{17}O [28].

3. Spin Dynamics

For the neutral charge state of the overall complex, the local environment of the muon is diamagnetic (i.e. there is no interaction with unpaired electron spins). The spin dynamics is then governed by the Hamiltonian [2]

$$H = H_Z + H_Q + H_D \tag{1}$$

where H_Z denotes the interaction of the boron spin J and the muon spin I with the external field B :

$$H_Z = -\hbar\gamma_J \boldsymbol{J}\cdot\boldsymbol{B} - \hbar\gamma_I \boldsymbol{I}\cdot\boldsymbol{B} \tag{2}$$

giving rise to the Zeeman frequencies $\omega_J = \gamma_J B$ and $\omega_I = \gamma_I B$, respectively. The quadrupole interaction of the boron spin due to an electric field gradient directed along the unit vector $\boldsymbol{n}$ is given by

$$H_Q = \hbar\omega_Q \left[(\boldsymbol{n}\cdot\boldsymbol{J})^2 - \tfrac{1}{3}J(J+1)\right] \tag{3}$$

where

$$\omega_Q = 3QV_{zz}/4J(2J-1). \tag{4}$$

The dipolar interaction H_D between the boron and the muon is

$$H_D = \hbar\omega_D\,(\boldsymbol{I}\cdot\boldsymbol{J} - 3(\boldsymbol{n}\cdot\boldsymbol{I})(\boldsymbol{n}\cdot\boldsymbol{J})) \tag{5}$$

with

$$\omega_D = \hbar\gamma_J\gamma_I/R_{I-J}^3. \tag{6}$$

Owing to the weakness of the dipolar interaction, a muon polarized initially in the direction of the external field $\boldsymbol{B}$ will in general not change its polarization (spin-lattice relaxation is expected to be negligibly slow on the timescale of the muon lifetime). Exceptions occur at very small fields and around those field values where the energy separation of the Zeeman levels of the muon ($\hbar\gamma_I B$) is equal to that of adjacent quadrupole energy levels of the boron nucleus ($\hbar\omega_Q(2m_J - 1)$). At these resonance fields the boron–muon dipole–dipole interaction leads to an exchange of polarization between the muon and the boron nucleus. Since the lifetime of the muon ($\tau_\mu = 2.2\ \mu s$) is much smaller than ω_D^{-1}, an apparent depolarization of the muon is observed. The details of this mechanism can be demonstrated if the direction of the external field coincides with the direction of the field gradient, as in this case an analytic solution is possible [31]. With the help of the abbreviations

$$R_m = \omega_D\sqrt{J(J+1) - m(m-1)} \tag{7}$$

$$S_m = (2m-1)(\omega_Q + \omega_D) + \omega_J - \omega_I \tag{8}$$

the longitudinal muon polarization can be written as

$$p(t) = \frac{1}{2J+1}\left(1 + \sum_{m=-J+1}^{J} \frac{1}{R_m^2 + S_m^2}\left[S_m^2 + R_m^2\cos(\sqrt{R_m^2 + S_m^2}\,t)\right]\right). \tag{9}$$

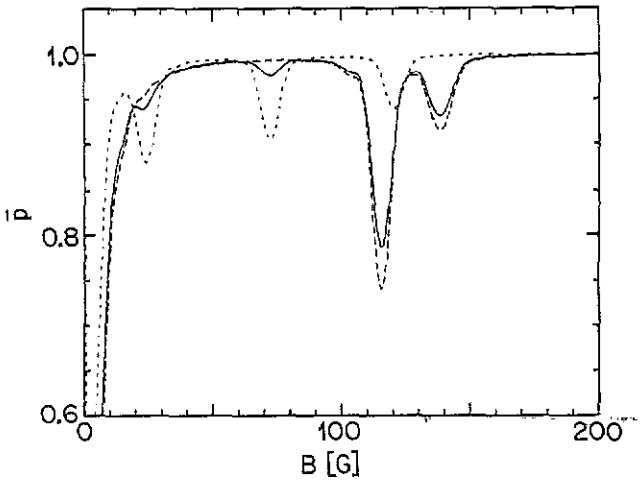

Figure 2. Integrated polarization curve $\bar{p}$ as a function of field along the ⟨100⟩ direction. The dashed curve is for ^{11}B (spin 3/2), the dotted one for ^{10}B (spin 3). The solid line is a mixture of these contributions according to the natural abundancies.

For most field values the amplitudes of the oscillating terms are negligible since $S_m^2 \gg R_m^2$. If S_m vanishes, however, the amplitude of the corresponding oscillating term becomes significant and for short times an apparent depolarization sets in.

For the particular case of a spin $J = 3/2$ nucleus, the resonance field is $B_r = \gamma_I^{-1}(2(\omega_Q + \omega_D) + \omega_J)$ and the corresponding time dependence of the muon polarization at B_r is given by

$$p(t) = \tfrac{1}{4}[3 + \cos(\sqrt{3}\omega_D t)]. \tag{10}$$

The positions of the resonances are governed by the boron quadrupole coupling constant, i.e. by the electric field gradient experienced by the boron nucleus. For the model depicted in figure 1, this is found (table 1) to be

$$V_{zz} = -0.376 \text{ au}. \tag{11}$$

So for the more abundant isotope ^{11}B, using the value $Q = 12.7 \times 10^{-10}$ au for the electric quadrupole moment [32]

$$Q = 12.7 \times 10^{-10} \text{ au} \tag{12}$$

we obtain for the quadrupolar parameter the value

$$\omega_Q = -4944 \times 10^3 \text{ s}^{-1}. \tag{13}$$

This leads to a transition frequency in zero field of $2\omega_Q/(2\pi) = 1.57$ MHz and to μLCRs in the vicinity of $2\omega_Q/(\gamma_\mu - \gamma_B) \approx 130$ G, the exact positions depending slightly on orientations. Likewise the dipolar parameter, also for ^{11}B, is

$$\omega_D = 229 \times 10^3 \text{ s}^{-1} \tag{14}$$

leading in the case of the external field being applied along the ⟨111⟩ direction to an oscillatory exchange of polarization on resonance with frequency $\sqrt{3}\omega_D/(2\pi) =$ 63 kHz.

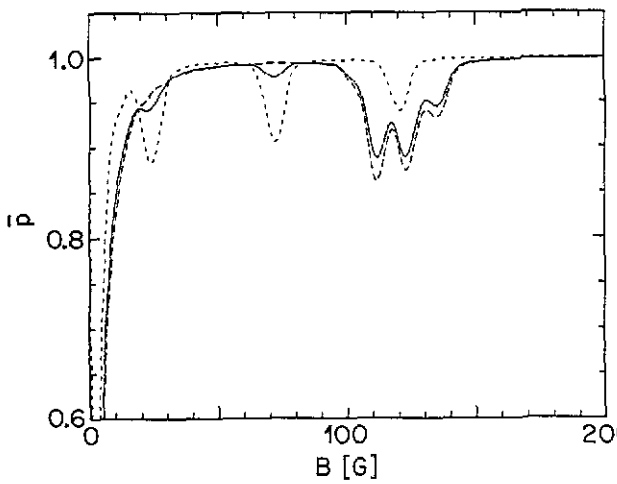

Figure 3. Integrated polarization curves as a function of field along the ⟨111⟩ direction, with definitions as in figure 2.

The detailed predictions for the positions and amplitudes of the resonances are given in figures 2 and 3, for the bond-centre configuration of the complex. In this presentation, residual muon polarization is displayed, integrated over a time window which is delayed relative to the muon implantation so that the exchange of polarization has an appropriate time to develop:

$$\bar{p} = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} \mathrm{d}t \; p(t) \tag{15}$$

with $t_1 = 3$ μs and $t_2 = 10$ μs. This is also a particularly convenient form in which to present data from a pulsed muon source. In figure 2 the results of calculations for the external field along the ⟨100⟩ direction are given for both isotopes ^{10}B and ^{11}B and in figure 3 for the field along ⟨111⟩. It is noteworthy that in experiments in which integral positron counting is employed, e.g. at intense continuous muon sources, the resonances would appear somewhat smaller in amplitude (by about a factor of 3 in the present example), such data being weighted to early times by the muon decay, according to

$$\int_0^{\infty} \mathrm{d}t \; p(t) \; \exp(-t/\tau_\mu).$$

(The signal-to-noise ratio can be maintained, however, by an appropriate level of statistics.) For a comparison of these predicted resonances with possible experiments one has to be aware of the fact that these resonances would be superimposed on the repolarization curves of the paramagnetic muonium fractions (i.e. Mu*, together with any untrapped Mu', the Mu* fraction dominating the field dependence in this region at low temperatures [3]). In figures 4 and 5 the results of calculations are therefore presented in which various admixtures or fractions f^* of muons which form Mu* centres without having B nuclei as nearest neighbours have been taken into account. (Note that for about 9% of the intrinsic Mu* centres one of the neighbouring Si atoms is ^{29}Si, for which a superhyperfine interaction has been determined by Kiefl *et al* [5]. Inclusion of the interaction parameters for these centres in the calculation

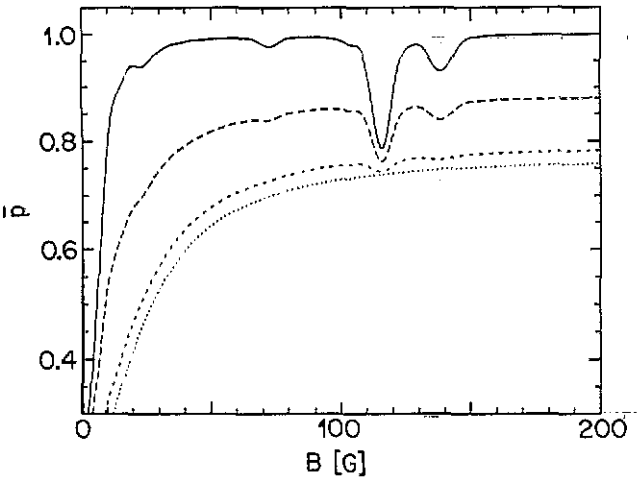

Figure 4. Integrated polarization curve $\bar{p}$ *as a function of field along* the ⟨100⟩ direction for admixtures of Mu* with fractions f^* of 0 (solid line), 50, 90, and 100% (dotted line).

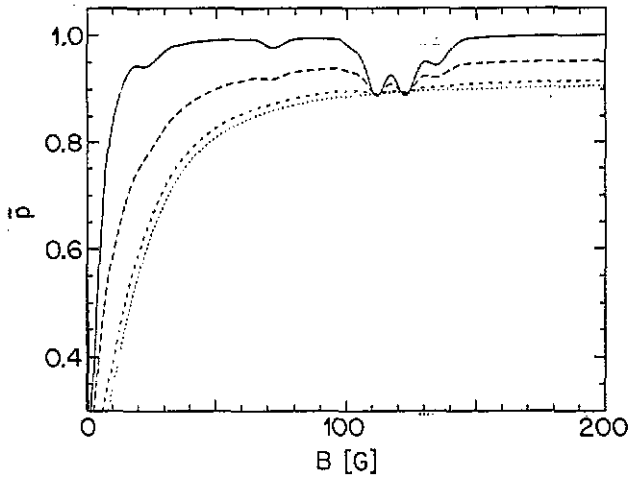

Figure 5. Integrated polarization curves as a function of field along the ⟨111⟩ direction, with definitions as for figure 4.

results in repolarization curves which differ only imperceptibly, however, from those of figures 4 and 5).

Electric field gradients at the boron nucleus for the metastable muon sites have also been calculated. The corresponding level crossing resonances fall in the region of 40 G (boron antibonding configuration) and 150 G (silicon antibonding configuration), well clear of the resonances expected for the stable complex. In fact, the greater boron–muon separation in the silicon antibonding configuration make this resonance so weak that it is undetectable. The situation for diamagnetic complexes therefore contrasts markedly with that for paramagnetic centres, in which cross relaxation is typically much faster, and mediated over quite large separations by hyperfine couplings with the unpaired electron [33]. μLCR would therefore be unsuitable for the detection of passivation complexes with donors such as As (note that P in any case has no quadrupole moment), for which the stable muon site is not expected to be immediately adjacent to the defect.

4. Experimental considerations

In our exploratory experiments performed to date we have not been able to detect the well resolved resonances predicted. These experiments were performed mainly at ISIS (pulsed muon source), with some additional tests performed at TRIUMF (continuous muon source). For the ISIS experiments silicon wafers with ⟨111⟩ orientation were available to us, with boron doping varying from moderate ($[B] = 2\times 10^{17}$ cm^{-3}) to very low (high purity silicon, $[B] < 10^{12}$ cm^{-3}). In fact, experiments with the applied field along the ⟨111⟩ direction are less than ideal in several respects: firstly, the expected boron resonance is split by the two inequivalent orientations of the passivation complex, as in figures 3 and 5; secondly, there is the possibility of confusion with a resonance representing the paramagnetic Mu* centres, i.e. muonium trapped at intrinsic bond-centre sites. This latter is the so called zero–crossing resonance at which $\Delta M = 1$ transitions of the muon spin alone become allowed when the applied field is not perfectly aligned with a Mu* symmetry axis; this resonance also lies close to 100 G [5] but, unlike those of the diamagnetic complexes, does not involve any neighbouring nuclear spins. μLCR scans performed at 20 K did indeed reveal a broad dip in the Mu* repolarization curve which must be assigned to the zero-crossing resonance: the presence of this feature in data for all samples, irrespective of boron concentration, confirms its association with intrinsic Mu* centres rather than with the passivation complexes.

No resonances which could be assigned unambiguously to boron were detected in the spectra of the p-type samples. (Some tantalizing indications of additional features closer to 200 G were recorded but we are unable at present to attach any significance to these: the departures from the Mu* repolarization curve are too weak to permit comparison with the ^{10}B/^{11}B isotopic signature of figure 5; they also appear at the same level as artefacts caused by occasional beam instabilities.) This is disappointing, and raises questions as to whether the complexes are formed with adequate probability on the scale of the muon lifetime, or whether the resonances are otherwise obscured. Consider first that the complexes are formed by the encounter of muonium with boron, both initially in the neutral charge state, as in process (16):

$$\text{B–Si} + \text{Mu} \longrightarrow \text{B–Mu–Si}. \tag{16}$$

The normal muonium or Mu′ fraction is known to be highly mobile at all temperatures in pure and lightly doped silicon, and is therefore able to explore the lattice. Hop rates (from one interstitial site to the next) in excess of 10^{12} s^{-1} are commonly quoted [3]. Diffusion limited trapping by defects with a trapping radius of the same order as the lattice constant would therefore be effective on the microsecond timescale at defect concentrations of parts per million (5×10^{16} cm^{-3} in Si) and effects on muonium relaxation attributable to encounter with impurities are indeed observed at doping levels of 10^{14} cm^{-3} and above [34]. At low temperatures (below about 50 K) doping dependent relaxation is seen only in the transverse field spectra, and not in longitudinal field; it is therefore taken to represent dephasing rather than a loss of polarization due to spin-flip processes. This is encouraging for the present purpose; however, it is impossible to tell from this data whether an encounter also results in trapping. In the case that the trapping is activation limited, rather than diffusion limited, it may not be sufficiently effective on the time scale of the muon lifetime. This is a possible consequence of the significant displacement of the boron

atom in the structure depicted in figure 1 from its normal substitutional site: the local distortion of the lattice implies an energy barrier to formation of the complex which thermalized muonium may be unable to supply. Complexes in which the muon, for whatever reason, adopts a metastable site significantly further from the boron nucleus are not expected to be detected, the strength of the cross relaxation varying with distance as r^{-6}.

Some additional experiments performed at ambient temperature—a convenient condition at which the boron is largely ionized—also failed to detect the resonances. These experiments were performed at TRIUMF (M13 beamline) and included a sample doped to $[B] = 4 \times 10^{16}$ cm^{-3} and having the more favourable ⟨100⟩ orientation in which all the complexes are equivalent. Experiments at still higher temperature might be worthwhile, providing significant ionization of Mu′ as well as of B and favouring formation of the complexes via process (17). Here the initial as well as final states are diamagnetic, which should minimize any danger of the muon depolarizing prior to trapping. Process (17) could conceivably result in more efficient trapping, assisted by electrostatic attraction; dissociation of the complex is not expected below about 200 °C [19].

$$B^{-}\text{–Si} + Mu^{+} \longrightarrow \text{B–Mu–Si}. \tag{17}$$

Assuming that the complexes are formed, there is the interesting question of whether the muon moves rapidly between the four equivalent sites adjacent to the boron atom. This would render μLCR detection impossible even if the complexes were formed quickly: such a motion would wash out the resonances both by reducing the quadrupole splitting on boron to zero (the result of effective cubic symmetry) and by similarly averaging the dipolar coupling which drives the cross relaxation (a property of the traceless Hamiltonian). The effective barrier height of 0.19 eV deduced by Stavola *et al* for reorientation of the Si(B,H) passivation complexes [17] suggests that this is indeed possible, since the zero point energy of the muon will be greater than that of the proton by at least this amount. Stoneham has pointed out that the Si(B,H) data are in fact consistent with a tunnelling motion of the proton which is phonon assisted [35] and Ong and Khoo [36] go so far as to suggest that the proton may be delocalized over a considerable portion of a spherical shell (radius 1.22–1.25 Å) around the boron.

Any such process will certainly be faster for the lighter muon. There is also the possibility of a coherent tunnelling state in which the muon occupies the four sites with equal probability and the boron remains in this case undisplaced from its central position. This would imply that in this situation the muon is not quite heavy enough to self-trap within a particular bond in the same manner as the proton [37]. If this proves to be the case, resonances similar to those of figures 2–5 would only be detectable if a means can be found to induce self-trapping by breaking the local symmetry, e.g. with the aid of additional impurities or via the application of uniaxial stress.

There is also a good chance that μLCR would be detectable in p-type amorphous silicon, a-Si:B. The positions of the resonances are only weakly dependent on the orientation of the complexes but the randomness of the structure should be sufficient to prohibit their fast reorientation.

All these considerations point to the need for μLCR studies to be pursued over a wider range of sample conditions and we plan further experiments aimed at establishing conditions favourable to detecting the spectra. High doping levels would seem

most promising, although no attempt has yet been made to model this situation e.g. to investigate how the overlapping wavefunction of a neighbouring unpassivated acceptor may influence the configuration of figure 1, or otherwise modify the quadrupole resonance spectra.

The possibility of performing a conventional NQR experiment on highly doped Si(B,H) should also not be overlooked, the complexes in this case being preformed and their reorientation rate negligible at low temperatures. Here the limitation is instead the sensitivity of detection. The quadrupole resonance frequencies are as predicted in section 2, but their direct detection would be extremely difficult in view of the small magnetic moment of the boron nuclei. A more promising approach would seem to be detection via the protons using double resonance or cross relaxation spectroscopy [38], the proton magnetisation being measured on return from the resonance condition to a suitably high magnetic field. With this difference in the detection technique, the muon and proton experiments are closely analogous and should result in very similar spectra; for protons the resonant fields will be higher by a factor of approximately 3 (i.e. by the ratio of the magnetic moments of muons and protons, with due allowance for the small Zeeman energy of the boron nuclei). If samples can be prepared with passivation complexes present at the level of $[B] \geqslant 10^{19}$ cm^{-3} (i.e. $\geqslant 0.05$ atomic percent hydrogen), such a study should be feasible.

Acknowledgments

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