Far-infrared spectroscopy of P ion-implanted Si

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Abstract

The spectroscopy of impurity atoms in elemental Si has a long history and has received a fillip in recent years with the development of the Kane quantum computer. In this study we report on one method of incorporating P (and P dimers) into the semiconductor host lattice, namely ion-implantation, and one method of analysing for the impurity, namely far-infrared magnetospectroscopy. A bulk, neutron-transmutation doped sample was used as a reference material, as was a bulk, growth-doped sample of higher impurity concentration. A dimer-implanted sample and a heavily-doped implanted sample were then investigated. The bulk samples show spectral lines similar to those observed previously, although the lines were greatly broadened in the case of the more highly doped sample. The two ion-implanted samples did not exhibit any phosphorous transition lines. The reasons for this are discussed.

Introduction

In the prototypical semiconductor, silicon, the classic donor impurity is phosphorus. The archetypal system of Si(P) has consequently been extensively investigated, with studies stretching back half a century; for example, Pearson and Bardeen (1949).

Interest in the system Si(P) received a tremendous stimulus about ten years ago when Kane proposed a silicon-based quantum computer (Kane 1998; see also Skinner *et al.* 2003). The Kane paper has been cited more than 1700 times and has led to an explosion of activity around the world. To give but one recent example, McKamey *et al.* (2008) have investigated spin-dependent processes at the Si(P)-SiO_2 interface with a view to demonstrating the feasibility of reading out donor qubits.

The incorporation of P into Si may be accomplished by many methods. These include growth from the melt and neutron-transmutation doping (NTD). The use of ion implantation has been proposed for applications in quantum computation as the depth of the P below the surface may be readily controlled and the implantation of P dimers immediately yields adjacent P sites. In this study, we investigate ion-implanted P in Si.

A number of techniques are available to examine the state of P in Si; for example, electron spin resonance (Bulatovic *et al.* 2008). A very sensitive method for probing impurity state is far-infrared absorption spectroscopy. According to the effective-mass theory, the shallow substitutional donor impurity forms a hydrogen-like system. The effective Rydberg Ry^* is given by scaling the usual Rydberg Ry using the effective mass of the electron, m_e, and the dielectric constant of the host lattice, $\epsilon(0)$: $Ry^* = m^* Ry/(m_e \epsilon(0)^2)$. Analogous to the spectroscopic series of transitions observed in the hydrogen atom, such as the Lyman series, spectroscopic absorption lines are observed for Si(P). In view of the smaller effective mass of the electron in Si(P) relative to in the vacuum, and the larger dielectric constant, the effective Rydberg is much smaller, and so the transition energies are much smaller, being observed in the far-infrared, rather than the visible. In fact, a particular transition of Si(P), the $1s \to 2p_0$ transition, is observed to be very sharp (Jagannath *et al.* 1981) and in isotopically-pure ^{28}Si is the sharpest of any impurity transition reported for any semiconductor (Karaiskaj *et al.* 2003). In this investigation we employ far-infrared spectroscopy to probe the Si(P) donor states.

Our original measurements on the ion-implanted samples, carried out using a Bomem DA3.26 spectrometer, failed to show any absorption features characteristic of the transitions associated with P in Si. It is well known that in other systems, for example for donors in GaAs (Stillman *et al.* 1969), that the application of magnetic field strongly enhances the spectral transitions. For this reason, it was decided to conduct further experiments, which are reported here, in a strong magnetic field.

Materials and Methods

Details of the samples used in this research are set out in Table 1. Apart from the ion-implanted samples, two bulk Si(P) samples, one of "light" doping ($n = 1 \times 10^{14}$ cm^{-3}) and one of "heavy" doping ($n = 8 \times 10^{16}$ cm^{-3}) were examined by way of comparison. The back faces of the samples were wedged to suppress interference fringes between the front and back surfaces.

Table 1: **Summary of the Si(P) samples employed**

	SiPRL3A	SiPB	SiP4	SiP5
doping	bulk	bulk	implanted	implanted
details	NTD	0.1 Ω-cm	16 keV P$_2$	180 keV
thickness (μm)	1588	262	333	326
n_{3D} (cm^{-3})	1×10^{14}	8×10^{16}	–	–
n_{2D} (10^{12} cm^{-2})	16	2096	5	100

The far-infrared spectroscopy was carried out using a Bruker 113 V rapid-scan Fourier spectrometer. Appropriate radiation sources and filters were chosen to allow a wide spectral range to be examined. Data were taken with the sample at 4.2 K. Most spectra were taken at a resolution of 0.5 cm^{-1}, some at 2 cm^{-1}. The light was conducted from the spectrometer to the field centre by a light pipe. The magnetic field was provided by a superconducting solenoid. The magnetic field was parallel to the propagation direction of the light from the spectrometer (that is, the Faraday geometry was employed). The light was nominally unpolarised. A helium-cooled Si bolometer served as the radiation detector.

Results and Discussion

Bulk samples
Spectra for the bulk samples are presented in Figures 1 and 2. They are shown for each sample at zero magnetic field and at magnetic field of 18 T. The zero field data is absolute transmission; the 18 T data appears more transmissive due to the magnetoresistivity of the detector, which has not been corrected for here as it provides a convenient offset. The very sharp lines in the spectrum are due to water vapour; these do not completely ratio out from the reference (no sample) spectrum.
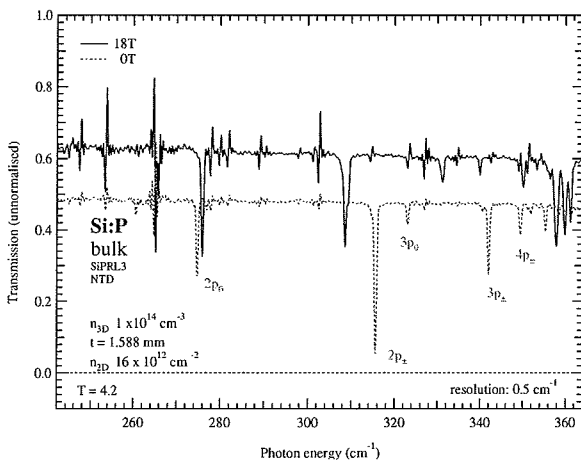

Figure 1: Spectrum of a "lightly" doped sample of Si(P) in both zero magnetic field (bottom, dashed, red line) and in magnetic field of 18 T (top, full, blue line).
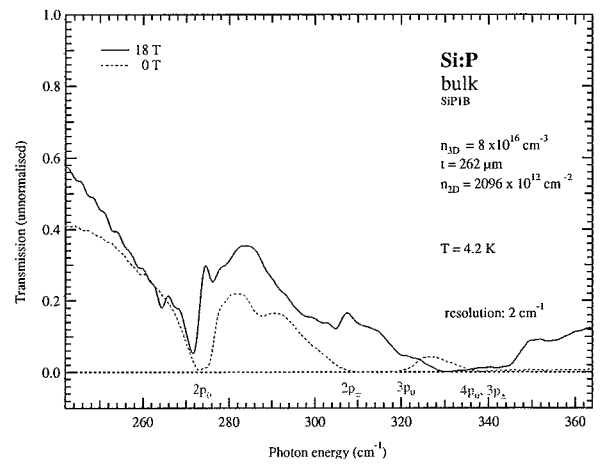
Figure 2: Spectrum of a "heavily" doped sample of Si(P) in both zero magnetic field (bottom, dashed, red line) and in magnetic field of 18 T (top, full, blue line).

The "lightly" doped sample of Si(P) exhibits sharp spectral lines in the absence of applied magnetic field (Figure 1). These arise from transitions from the $1s$ ground state to excited states, such as the $2p_0$, $2p_\pm$, $3p_0$, $3p_\pm$, and so on. The data of Figure 1 is in excellent agreement with the unperturbed spectrum previously observed by others, for example Jagannath et al. (1981). The application of a magnetic field causes the lines to shift and split, as is evident from the spectrum shown at 18 T. The details of the development of the spectral lines with field will not be discussed further here; the interested reader may refer to Mu et al. (1993) and Shen et al. (1994), which deal with the development to 10 T, and to Lewis et al. (2005), which extends the field to 18 T.

The "heavily" doped sample, Figure 2, exhibits much deeper and broader lines in transmission. For instance, the $2p_0$ line is almost black; the $2p_\pm$ and $3p_0$ lines are merged at zero field, as are the $3p_\pm$ and $4p_0$ lines. The line positions are also slightly shifted relative to the less-heavily doped sample. These effects of (a) concentration broadening and (b) change in the ionisation energy with doping are well known. On the application of magnetic field, the spectral lines again shift and split. In this particular example, our detailed (unpublished) data at intermediate magnetic fields show both the development of Zeeman lines associated with the bound impurity levels, (as in the "lightly" doped sample), and also the development of lines associated with the Landau levels in the continuum. We believe the particular combination of relatively high doping and strong magnetic fields have made the observation of the Landau-related transitions possible.

Ion-implanted samples
Spectra for the ion-implanted samples are given in Figures 3 and 4. As for the bulk samples, spectra are shown for each sample at zero magnetic field and at magnetic field of 18 T. The high-field data is again offset due to the magnetoresistance of the detector.
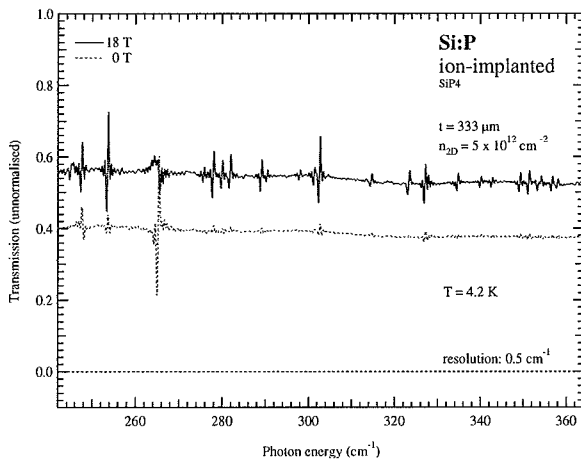

Figure 3: Spectrum of an ion-implanted dimer sample of Si(P) in both zero magnetic field (bottom, dashed, red line) and in magnetic field of 18 T (top, full, blue line).
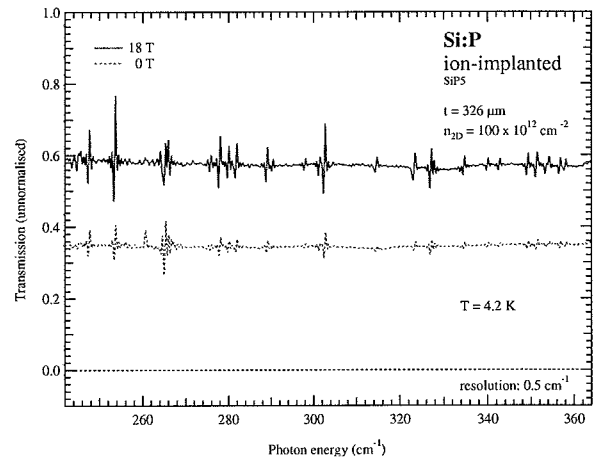
Figure 4: Spectrum of an ion-implanted sample of Si(P) in both zero magnetic field (bottom, dashed, red line) and in magnetic field of 18 T (top, full, blue line).

It may be seen in Figures 3 and 4 that the two ion-implanted samples do not exhibit any transitions associated with excitation from the $1s$ state of P in Si. The only features appear to be the sharp spikes related to the incompletely-ratioed water vapour, as mentioned previously. In particular, there is no evidence of the strong $1s \rightarrow 2p_0$ or $1s \rightarrow 2p_\pm$ transitions. This is the case both without applied magnetic field and also in the strong applied magnetic field of 18 T.

Comparison of bulk and ion-implanted samples
The Si(P) lines are clear in both bulk samples but not evident in either ion-implanted sample. The question arises as to why this should be. Whether the ion implantation is at relatively low energy (16 keV, Figure 3) or relatively high energy (180 keV, Figure 4) does not seem to play a role. Likewise, whether dimers (Figure 3) or monomers (Figure 4) are implanted seems to make no difference. It may be thought that the sensitivity of the experimental method is too poor to detect the small number of implanted ions. Absorption spectroscopy is sensitive to the total number of absorbing centres through which the beam passes, regardless of how they are spread along the beam length. In this circumstance, we can calculate the equivalent two-dimensional density of P atoms in the bulk samples (knowing their bulk density and thickness) and compare this with the assumed two-dimensional density of the implanted P atoms;

this data is given in Table 1. It might appear that the 2D concentration of P atoms in sample SiP4, being the lowest of the four samples examined here by a factor of about 3, might be too low to be detected. An inspection of Figure 1 shows this not to be the case, as, for example, the $3p_0$ and $4p_\pm$ lines are clearly observed in the "lightly" doped sample, in spite of being much less than one-third of the strength of the strongest, $2p_\pm$ line. The method is clearly sensitive enough to detect the concentration of P atoms in sample SiP5, as this falls midway between the two bulk sample, both of which show the expected spectral lines.

We consider that the most likely explanations for the lack of observed lines is either that the P atoms are not substituting perfectly for the Si atoms, so forming interstitial or other non-hydrogenic structures, or that the post-implantation annealing is insufficient to relieve all the damage caused to the lattice in the process of implantation, or a combination of these factors. This result and explanation is not inconsistent with the data presented from electron spin resonance (Bulatovic *et al.* 2008) where a diminished P signal was attributed to the presence of charge traps.

Conclusions
We have compared the far-infrared spectra of bulk and ion-implanted samples of P in Si in both zero and high (18 T) magnetic field. The bulk samples show the expected hydrogen-like transitions, suffering concentration broadening as the doping level increases. Neither ion-implanted sample shows these transitions. The absence of the lines does not appear to be directly related to whether the ion implanted is a monomer or dimer, or whether the implantation energy is large or small, but rather to the imperfect substitution of the P on Si sites or imperfections in the host lattice.

Acknowledgements

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