

Proceedings of the XXII International School of Semiconducting Compounds, Jaszowiec 1993

ON THE SYMMETRY OF THE SULFUR-PAIR-RELATED DEFECT IN SILICON

M.T. BENNEBROEK^a, A. ZAKRZEWSKI^b, A.M. FRENS^a AND J. SCHMIDT^a

^aHuygens Laboratorium, P.O. Box 9504, 2300 Leiden, The Netherlands

^bInstitute of Physics, Polish Academy of Sciences
Al. Lotników 32/46, 02-668 Warszawa, Poland

A sulfur-related-pair defect in silicon has been studied with optically detected magnetic resonance spectroscopy. Measurement of the angular dependence of the optically detected magnetic resonance signals supplemented by the analysis of the spectrum "quality" yield to the conclusion that the point group symmetry of the defect studied is C_{1h} .

PACS numbers: 76.30.Lh, 71.55.Ht

1. Introduction

Recently a sulfur-related complex defect in silicon has attracted much attention due to its interesting configurational metastability [1–3]. Two photoluminescence spectra S_A and S_B , corresponding to two different geometric configurations of this complex dominate at low temperatures ($T < 10$ K) with zero-phonon lines S_A^0 and S_B^0 at 0.968 eV and at 0.812 eV, respectively. It has been shown [2] that these lines originate from photo-excited triplet states of an exciton bound to this defect in its neutral charge state. The first step in analyzing metastability is, of course, determination of the point group symmetry of a given defect. This is usually done via examination of the angular dependence of the magnetic resonance signals related to the defect.

The angular dependence of the optically detected magnetic resonance (ODMR) spectrum of S_A^0 was analyzed by Chen et al. [4] with a spin Hamiltonian

$$\hat{H} = \vec{S} \vec{D} \vec{S} + \mu_B \vec{S} \vec{g} \vec{B} + \vec{S} \vec{A} \vec{I} . \quad (1)$$

It was found [4] that the symmetry of the defect, giving rise to S_A spectrum, is monoclinic (C_{1h}), as shown in Fig. 1. The z axis is 17 degrees off $\langle \bar{1}11 \rangle$ towards $\langle 001 \rangle$ in the $[110]$ plane, y is parallel to $\langle 110 \rangle$ and x is perpendicular to both y and z . Since there are 4 inequivalent $\langle 111 \rangle$ axes and 3 inequivalent $\langle 110 \rangle$ axes around each $\langle 111 \rangle$ direction, we end up with total of 12 possible defect orientations. On the contrary, results obtained by Watkins [5] yield to the conclusion that the x -axis

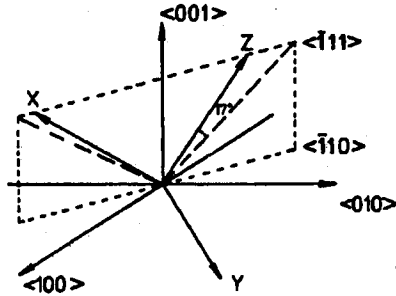


Fig. 1. The principal axes of the D -tensor. Note that in this figure there was adopted the normal ESR convention that the principal axis with the largest D -value is called z axis but not, as often used in the group theory convention, that in the C_{1h} symmetry the z axis is perpendicular to the mirror plane.

lies about 7 degrees outside the $[110]$ plane, whereas the z -axis coincides with that found by Chen et al. In this case, the symmetry is lowered to C_1 and a total of 24 orientations exist. An obvious limitation of both investigations was that the defect symmetry deduced from the angular dependence measurements only within one plane, namely $[110]$. Consequently, this large number of possible inequivalent defect orientations together with broad and overlapping resonance lines (Fig. 2a) enabled accurate ODMR studies of signal angular dependence.

In this communication we present detailed orientational study (i.e. not limited to the one particular plane) of the sulfur-pair-related defect in silicon giving rise to the S_A luminescence. The study enables us to determine the real defect symmetry. Moreover, we showed that the analysis of the "spectrum quality" can greatly improve an interpretation of the results of ODMR experiment. Here, we utilized the fact that ODMR signals are very sensitive to even small deviations of magnetic field from the high symmetry directions.

2. Results and discussion

The experiments were performed in a K -band spectrometer at 1.2 K. The samples (Si:S) were optically excited in a band from 800–1200 nm, selected with a set of filters placed in front of a 250 W halogen lamp. The S_A^0 phosphorescence was monitored in a region of 1200 to 1500 nm with a Northcoast EO817S or EO817L detector.

It was found that the z axis of the zero-field splitting tensor D is at 17 ± 3 degrees off $\langle 111 \rangle$ in the direction of $\langle 001 \rangle$ in the $[\bar{1}10]$ plane, in agreement with the previous results [4, 5]. The position of the x extreme could not be resolved. This can be easily understood via the simulation of the spectrum for one given orientation using values of the D -tensor which were determined from the previous zero-field ODMR experiments [6]. Remembering that around each $\langle 111 \rangle$ axis three equivalent z axes are positioned 17 degrees off this $\langle 111 \rangle$ and that simultaneously three x axes from other orientations are very close to $\langle 111 \rangle$ (see Fig. 1),

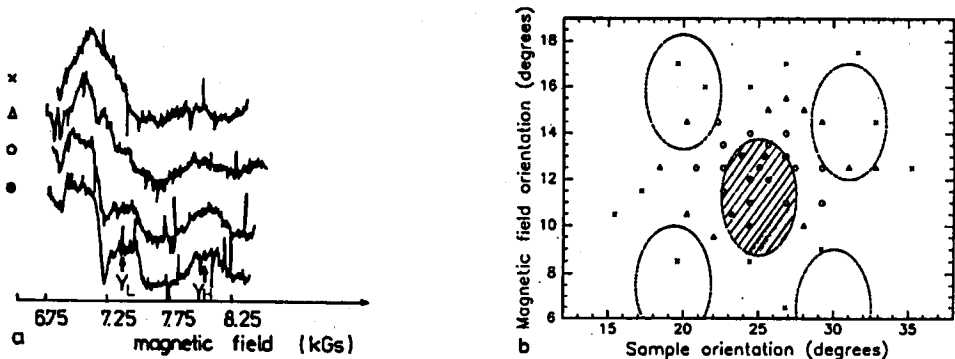


Fig. 2. (a) The four types of spectra on which we based our "mapping" method (i.e. making a "map" of the "spectrum quality" versus sample orientation). The low- and high-field transition are indicated by arrows. Definitions of the symbols: "●" displays what is assumed to be the "real" y spectrum, "o" displays a small deviation from "●". The low-field line partially overlaps with lower field transitions, whereas the high-field line starts to broaden. "Δ" displays a stronger deviation from "●" than "o". The low-field transition is just observable and the high-field line starts to split up into two lines. "x" displays every other shape. (b) A "map" of the "spectrum quality": hatched ellipse indicates the y direction according to Chen et al. [4] and open ellipses indicate the y directions according to Watkins.

the above mentioned z axes have contributions to the spectrum which, due to the very broad lines, overlaps with the x transitions. Fortunately, it was possible to find such other three orientations of magnetic field, which produce identical spectra as observed with B parallel to $\langle 111 \rangle$ direction. In this way, three equivalent $\langle 111 \rangle$ axes were found (i.e., $\langle \bar{1}11 \rangle$, $\langle 1\bar{1}1 \rangle$ and $\langle 11\bar{1} \rangle$). Then, these observations allowed us to construct all crystal axes, and, in particular we can predict the direction of $\langle 110 \rangle$ (hatched area in Fig. 2b).

The next step was to find position of the y axis. Unfortunately, y is a saddle point [6], and consequently cannot be determined in the same way as extreme positions are usually found. The method used here was to record the spectra around the predicted $\langle 110 \rangle$ axis and to characterize them by symbols showing their deviation from, what we believed to be an y -spectrum. In Fig. 2a four different categories of spectra are defined according to the number of lines, their width, shape and signal-to-noise ratio. The "best" spectra indicated by "●" have a width within 250–290 and 300–360 Gs for the low- and high-field transitions, respectively, and the spectra indicated by "o" have linewidths within 250–320 and 320–460 Gs, respectively. The obtained results based on that "spectrum quality" analysis are shown in Fig. 2b. In the same figure the expected direction of the $\langle 110 \rangle$ axis is indicated by the hatched ellipse. One can see that all the spectra indicated by "●" fall within the expected region of $\langle 110 \rangle$. This observation leads to the conclusion that y axis is really parallel to the $\langle 110 \rangle$ direction.

In Fig. 2b also the positions of the four y axes around $\langle 110 \rangle$, predicted by Watkins [5], are indicated by open ellipses. One can see that these positions clearly deviate from areas in which the y axes should lie according to our observations. It is this result of our conclusion that the sulphur-pair-related defect responsible for S_A luminescence has C_{1h} symmetry.

References

- [1] T.G. Brown, D.G. Hall, *Appl. Phys. Lett.* **49**, 245 (1986).
- [2] D.J. Beckett, M.K. Niessen, M.L.W. Thewalt, *Phys. Rev. B* **40**, 9816 (1989).
- [3] M. Singh, E.C. Lightowers, G. Davies, C. Jaynes, K.J. Reeson, *Mater. Sci. Eng. B* **4**, 303 (1989).
- [4] W.M. Chen, M. Singh, A. Henry, E. Jazen, B. Monemar, A.M. Frens, M.T. Bennebroek, J. Schmidt, K.J. Reeson, R.M. Williams, *Mater. Sci. Forum* **83-85**, 251 (1992).
- [5] G.D. Watkins, unpublished results.
- [6] A.M. Frens, M.T. Bennebroek, J. Schmidt, *Phys. Rev. B* **46**, 12316 (1992).