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PHOTOLUMINESCENCE FROM DEEP STATES ASSOCIATED WITH IRON IN SILICON

J. Weber[+] and P. Wagner[++]

[+]Physikalisches Institut der Universität Stuttgart
Pfaffenwaldring 57
[++]Max-Planck-Institut für Festkörperforschung
Heisenbergstr. 1
D-7000 Stuttgart 80
Federal Republic of Germany

The first investigation of photoluminescence in the spectral region between 1.2 and 1.7 μm of iron-doped *p*- and *n*-type silicon is reported. By Zeeman-splitting of the observed lines one can identify one cubic and two trigonal iron-related luminescence centers.

The properties of deep impurities in silicon are only scarcely known contrary to the well documented shallow donors and acceptors. One group of these impurities, the transition metal elements, show a complicated behavior. They exist in different charge states, occupy substitutional as well as interstitial lattice sites and form complexes with other impurities. The most important candidate of this group is iron. It forms a donor level 0.4 eV above the valence band [1,2]. This level has been identified by electron-spin-resonance as a neutral Fe ($3d^8$) on an interstitial lattice site. [3] Energy levels which are due to complexes of Fe and shallow acceptors have also been detected [2].

Luminescence is a powerful tool to study deep levels and has been successfully applied to II-VI- and III-V-compounds; silicon has thus far been less thoroughly investigated. We report here on luminescence of silicon doped with transition metals. From the observed luminescence lines and their Zeeman-splitting we deduce possible models for the Fe-related centers.

The samples used in the photoluminescence measurements have been prepared by diffusion of iron (copper) at 1100°C (850°C), followed by a rapid quenching of the samples in oil. The starting material was high purity *p*- or *n*-type float-zone silicon (10-300 Ωcm), cut into thin slices 300 μm thick. The Fe-concentration is in the range of 10^{15} cm^{-3} [4]. For the measurements the samples were cooled to liquid Helium temperatures.

We have investigated the luminescence of these samples in the spectral region from 1.0 to 2.0 μm. As shown in the upper part of Fig.(1) a broad luminescence band can be seen with a maximum at 0.7 eV and a halfwidth of 0.1 eV. This band is most intense in *n*-type samples, but can also be detected in *p*-type material. The high-energy side of this band starts at an energy of 0.73 eV, suggesting a transition of an electron to the interstitial Fe-level. On the high energy side of the band, groups of sharp lines can be seen. A very weak near-bandgap luminescence and in addition a group of lines at 1.22 μm is seen. These lines are associated with a copper-related complex, since they are particularly intense in deliberate-

ly Cu-doped samples. The remaining luminescence lines shown in the middle of Fig.(1) form three different groups centered at 1.4 μm, 1.6 μm and 1,7 μm. They are associated with Fe, as thermal quenched-in defects and other transition metal impurities were excluded by several null experiments. Some of these lines can also be observed in *p*-type samples (Fig.(1), lower part). The intensity of these lines is significantly lower in *p*-type samples than in *n*-type samples. An additional group of intense lines is seen in these samples in the near bandgap region at 1.16 μm.

We tentatively ascribe them to a recombination at Fe-B-pairs, as these centers can be made to vanish by shining white light on the samples at room temperatures. This behavior of Fe-B-pairs had been observed before in DLTS-experiments [4].

In the following we restrict ourselves to the group of lines at 1.4 μm, 1.6 μm, and 1.7 μm. We show that these lines are correlated with different Fe-centers. All three groups consist of sharp lines (half width ~0.1 meV) and broader equidistant low energy phonon replicas. The phonon energy seems typical for the Fe-correlated defects. The 1.6 μm and the 1.7 μm lines show the same phonon energy of 9.5 meV. The lines at 1.4 μm have a slightly higher phonon energy of 10.0 meV, which is also found for the lines tentatively correlated with Fe-B-pairs. In contrast to these observations, the

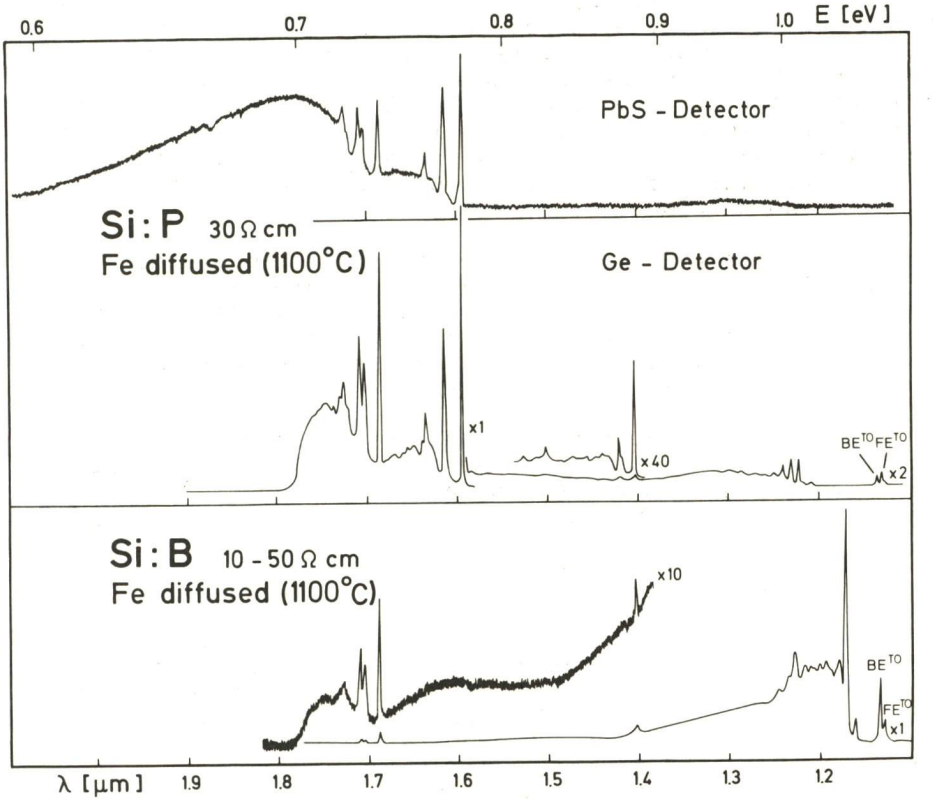

Fig.1 Photoluminescence spectra of Fe-doped silicon: Upper part *n*-type silicon, lower part *p*-type silicon

line group associated with Cu has a phonon energy of only 7.0 meV, but shows the same structure of a sharp zero phonon line followed by broader phonon replicas. One additional common feature of these lines is the increase in intensity with increasing shallow donor concentration in n-type samples and the independence from the chemical nature of the donor. Samples doped with phosphorous and arsenic show the same lines. From this beha ior we conclude, that the luminescent centers are in a neutral or negatively charged state.

At temperatures of ~20 K, excited states of the sharp zero phonon lines can be detected. These states differ clearly between the 3 line groups, indicating different electronic transitions for each group. The zero phonon lines associated with the line group at 1.6μm consist of two thermalising sharp lines at energies of 0.7766 eV and 0.7782 eV (±0.05 meV). These can be excited efficiently with a laser energy comparable to the bandgap of silicon. By using a Nd-YAG laser no bandgap luminescence was excited. In our thin samples only the 1.6 μm lines could be observed.

On the other hand, this line group could never be detected in p-type samples. For this reason, we propose for these lines an internal transition in a negatively charged Fe-complex. This assumption is supported by the Zeeman-splitting of these lines. Figure 2 shows the linear Zeeman-splitting of both zero phonon lines. The low energy line splits into 6 Zeeman components, while the higher energy line only shows a low-energy shoulder on a non-splitting line. The angular dependence of the Zeeman-splitting is nearly isotropic and can be described by assuming a cubic center.

The following level scheme explains the observed splitting very well: The ground state is fourfold degenerate with a g-value corresponding to cubic symmetry around the center. The excited states consist of two levels. The lower one is twofold degenerate with an isotropic g-value, the higher one has a fourfold degeneracy with the same angular dependence of the g-value as the ground state. The level scheme agrees with the assumption correlating these lines with internal transitions in a negatively charged interstitial Fe.

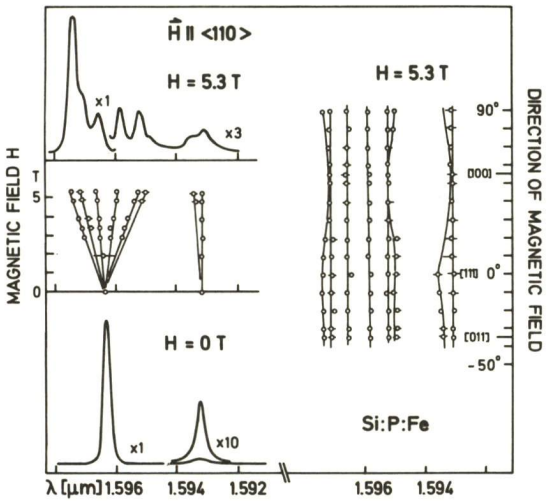

Fig.2 Zeeman-splitting and angular dependence of the zero phonon lines at 1.6 μm

The lines at 1.4 and 1.7 μm are preferentially excited with a laser energy higher than the bandgap of silicon. There are three thermalising zero phonon lines at 0.8819 eV, 0.8830 eV and 0.8834 eV (± 0.05 meV) in the 1.4 μm line group and two in the 1.7 μm region at 0.7343 eV and 0.7349 eV (± 0.05 meV). The Zeeman-splitting of these lines is nonlinear and anisotropic in all cases, the axis of symmetry corresponding to a <111> lattice direction. A detailed model to explain the nature of these luminescence lines does not exist at the moment. We favour a model of an exciton bound to an axial Fe-complex, the axis being determined by a nearest neighbour impurity or a Jahn-Teller distortion. This question of the orientation of the axis needs further investigations.

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