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Pseudodonor character of silver in silicon

Ingrid de Maat-Gersdorf*, T. Gregorkiewicz, C.A.J. Ammerlaan

Van der Waals-Zeeman Laboratorium, Universiteit van Amsterdam, Valckenierstraat 65–67, NL-1018 XE Amsterdam, The Netherlands

Abstract

Silicon doped with silver has been studied by photoluminescence. The results are compared with the optical absorption spectra available for the same impurity and are found to be similar. Further, the spectra are compared with the data on pseudodonor systems in silicon and a pseudodonor behavior of the silver dopant is considered.

1. Introduction

Photoluminescence and optical absorption of many defects in silicon are observable in the near-infrared region. Some of these spectra can be readily interpreted within the so-called pseudodonor model.

In the pseudodonor model, an isoelectronic defect binds an exciton forming a system with a tightly bound hole and a loosely bound electron, which can be described with the effective-mass theory (EMT). In comparison to a conventional donor, a pseudodonor is then characterized by an additional deep level corresponding to electron–hole recombination. The presence of this level shifts the EMT series as observed in photoluminescence to considerably higher energies.

A well-documented example of a pseudodonor system is the C line (0.79 eV). Fig. 1(b) presents the photoluminescence excitation (PLE) spectrum as obtained for this center [1]. At somewhat higher temperatures of 20 K, a very complete spectrum can be seen: five 1s, the $2p_0$ and the $2p_\pm$, and four 2s lines can be readily distinguished. In the absorption spectrum (Fig. 1(a)) only the four 1s lines of the lowest energy can be seen [2]. Of the so-called 615 meV defect, another pseudodonor, only the absorption spectrum is known [3]. Also this spectrum shows the transitions to s states exclusively.

In this paper we discuss a recently reported photoluminescence (PL) spectrum of silver-doped silicon [4]. By comparing the PL and absorption spectra we postulate that the silver dopant in silicon represents a pseudodonor system.

2. Experimental results and discussion

Until recently the silver dopant in silicon has only been studied in deep-level transient spectroscopy (DLTS) and Fourier transform infrared (FTIR) spectroscopy. When introduced into silicon, silver gives rise to several electrical levels in the band gap. The DLTS measurements established an amphoteric character of the impurity with donor and acceptor levels at $E_d = E_v + 340$ meV and $E_a = E_v + 540$ meV, respectively.

In a study by FTIR and photo-thermal ionization spectroscopy (PTIS), Olajos et al. [5]

* Corresponding author.

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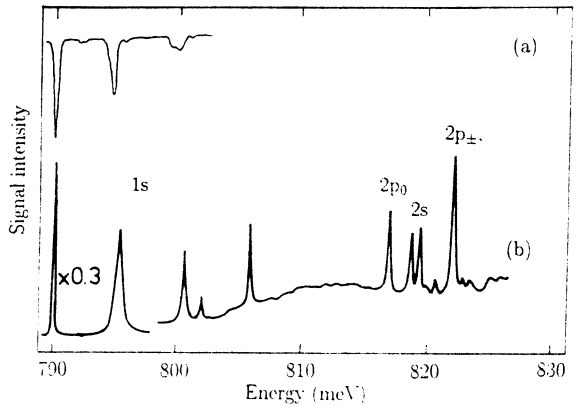

Fig. 1. (a) Infrared absorption spectrum of the C line (0.79 eV) in silicon by Foy [2], (b) photoluminescence excitation spectrum of the C line observed by Thonke et al. [1].

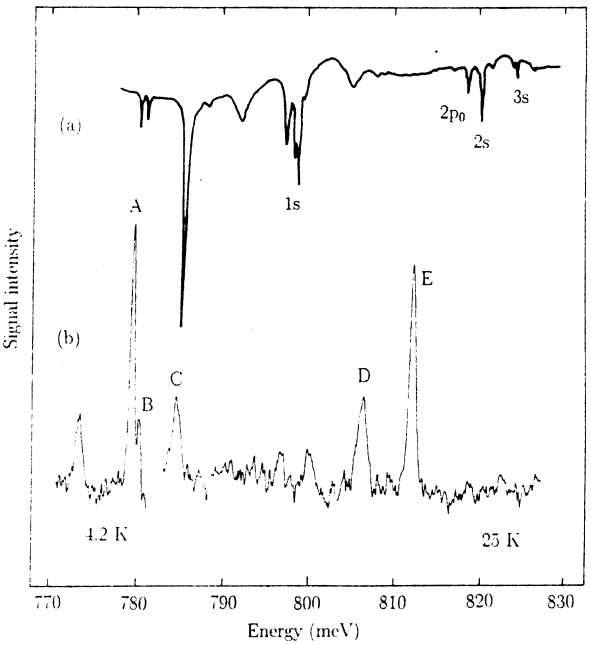

Fig. 2. (a) Infrared absorption spectrum of silver-doped silicon observed by Olajos et al. [5], (b) photoluminescence spectrum observed in silver-doped silicon at 4.2 and 25 K [4].

reported on a series of lines assigned to the neutral state of the isolated substitutional silver impurity. The spectrum, shown in Fig. 2(a), is dominated by the lines around 779 and at 784.5 meV which are identified as originating from many-particle and spin-orbit effects. The spectrum also shows transitions to 1s–3s states whereas practically no p-related transitions, which are characteristic for a donor, are visible. The identification of the spectrum was based on its comparison with spectra of effective-mass donors (phosphorus and tellurium) and further supported by its assumed similarity to the gold donor spectrum. This spectrum is dominated by excitations to s states. Svensson et al. compare the 615 meV absorption spectrum, the C line and this Ag spectrum and conclude that these spectra arise from pseudodonor-like defects [3].

Fig. 2(b) presents the PL spectrum as measured for a silver-doped sample, in the 770–828 meV range at 4.2 and 25 K. The experimental details of sample preparation and PL equipment will be presented elsewhere [4]. At 4.2 K three lines are detected: the two overlapping lines near 779 meV and a local phonon at 773.1 meV. Only at higher temperatures some more lines appear. As can be concluded by comparing Figs. 2(a) and 2(b), the silver-related spectra show great similarities, i.e., the A, B, and C bands and the local phonon of the same value. In addition, the PL spectrum shows two more prominent lines at 806.1 and 811.6 meV, labeled D and E, respectively. They are not seen at 4.2 K, while upon gradual increase of the temperature, the line at 806.1 meV appears first followed by the line at 811.6 meV whose intensity increases faster. These lines, which can be identified as two no-phonon lines with a separation of ≈ 5.5 meV accompanied by phonon replicas with LP value of 6.2 meV, do not find their equivalent in the absorption spectrum.

The experimentally evident correlation of appearance and the identical LP value argue for relating both sets of lines, as observed at low and higher temperatures, to (basically) the same center. The first possibility would be to examine whether all the absorption and PL lines can be understood within the energy scheme of a single system. Taking into account their mutual separation, lines D and E could readily be identified as transitions from the $2p_0$ and the $2p_\pm$ states whose appearance compares well with the PLE spectrum of the C line as referred to above and given in Fig. 1(b). The line E would correspond to an electron in its $2p_\pm$ state, while the D line would be a superposition of a transition

from $2p_0$ and an LP replica of the $2p_\pm$ line. The line at $\approx$ 800 meV would represent an LP replica of the $2p_0$ transition. Such an identification would require that at least some of the lines observed by Olajos et al. would have to be re-assigned to different transitions and the scheme would yield a very big central cell correction. Moreover, the intensity of the D and E lines clearly cannot be explained clearly by thermalization of the s states. In view of these arguments, proposing a single energy scheme for all the observed lines does not seem to be realistic.

Another possibility of explaining the experimental data is provided by assuming that upon laser excitation the silver dopant can form two centers of somewhat different electronic configuration, with the transformation between them being thermally activated. Similar bistability has been observed before for other impurities in silicon [6,7]. In one of these states silver would behave as a deep donor giving rise to excited states as observed both in absorption and PL. However, upon increasing the temperature, the formation of an isoelectronic bound exciton (IBE) would also become possible. The D and E lines would correspond to the ground state of such an IBE system with their temperature behavior characteristic for the singlet and triplet components split due to considerable j–j interaction.

Further studies are definitely necessary to confirm the bistability and a possible pseudodonor behavior of the silver dopant in silicon.

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