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PHOTOLUMINESCENCE STUDY OF THE 779-meV BAND IN SILVER-DOPED SILICON

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ABSTRACT

By means of photoluminescence the 779-meV band of silver-doped silicon has been studied. From temperature dependencies and comparison of our results with the published infra-red absorption data, we found that the spectrum observed around 779-meV energy can be identified with an isolated interstitial silver atom which exhibits pseudodonor character. This identification is in agreement with the Si-NL42 center measured by electron paramagnetic resonance in the same material.

INTRODUCTION

Silver, which belongs to the important life-time controlling impurities in silicon, has been studied by deep level transient spectroscopy [1], Fourier-transform infra-red absorption [2] and electron paramagnetic resonance (EPR) [3, 4]. Also some silver-related photoluminescence (PL) has been reported [5, 6].

Recently Son *et al.* [3, 4] studied silver-doped silicon by means of EPR. In a variety of samples, with different diffusion conditions, 6 silver-related centers were observed. EPR measurements performed on the material used in this study show the most prominent presence of the, so-called, Si-NL42 center which has T_d symmetry, and is identified with isolated interstitial silver.

The absorption spectrum of silver-doped silicon has been measured by Olajos *et al.* [2]. The spectrum shows a series of lines assigned to the donor level of the isolated, probably substitutional, silver impurity. The identification is based on its comparison to spectra of effective-mass donors, like phosphorus and tellurium, and supported by the similarity of its 1s band to that of the substitutional gold spectrum. The presented identification is less reliable because the p-lines series, which are characteristic for a donor, are practically missing.

DISCUSSION OF EXPERIMENTAL RESULTS

The photoluminescence spectrum of silver-doped silicon was observed at wavelengths between 1150 and 1750 nm, corresponding to an energy range of 1078 to 708 meV, and at temperatures of 4.2, 20, 30 and 40 K; the results are depicted in figure 1. The position of some lines in this spectrum, as indicated by a bold number, is also given in table I.

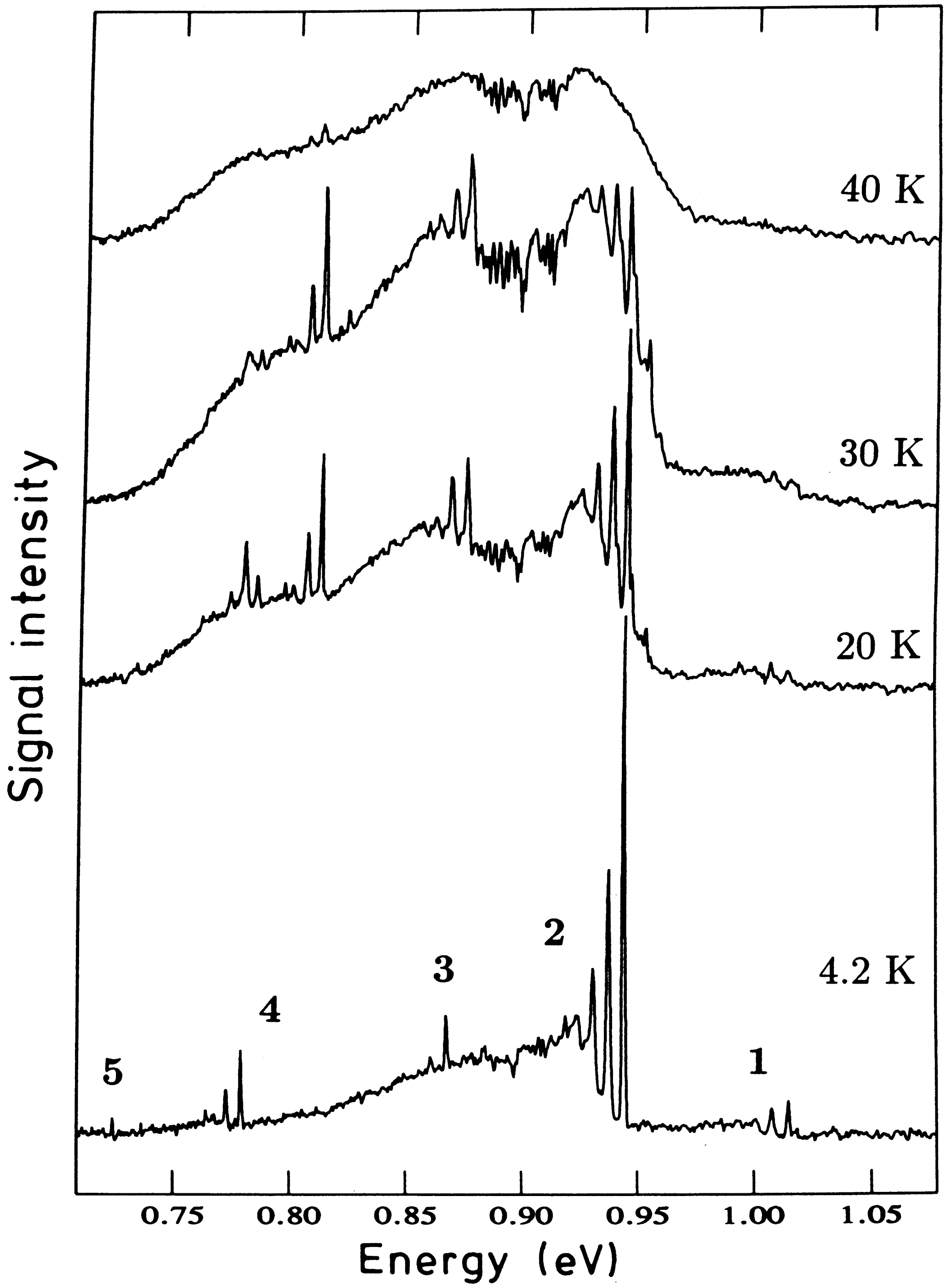

Figure 1: Photoluminescence spectrum of Si:Ag in the energy range 708 to 1078 meV, measured at 4.2, 20, 30, and 40 K. Luminescence bands are labelled by numbers 1 to 5.

Table I. Wavelengths and energies of the photoluminescence lines observed in silver-doped silicon. Spectral data are taken from figure 1. The temperature of the measurement is indicated.

line	wavelength (nm)	energy (eV)	temperature range (K)	assignment
1	1221.7	1.0149	< 50	Cu–Cu pair
2	1313.0	0.9447	< 50	Cu-related
3	1416	0.8756	15 - 50	Ag-related
	1429.0	0.8675	< 50	
	1438.9	0.8614	< 50	
4	1526.6	0.8116	11 - 60	Ag
	1537.1	0.8061	7 - 60	
	1546.5	0.8010	7 - 50	
	1555	0.7973	20 - 50	
	1559	0.7953	20 - 50	
	1580.5	0.7845	10 -40	
	1589.8	0.7799	< 40	
	1591.6	0.7790	< 40	
	1603.7	0.7731	< 30	
5	1690	0.7336	20 - 50	Ag-related
	1712	0.7242	< 30	
	1725	0.7188	< 30	

In figure 2 one finds the PL spectrum in the range of 770 – 828 meV at the temperatures of 4.2 and 25 K in more detail; also the absorption spectrum found by Olajos *et al.* [2] is depicted, showing a close similarity. At 4.2 K three different lines are easily detected; the two overlapping lines near 779 meV correspond to the lines A and B from the absorption spectrum. Moreover, there appears at least one local-phonon (LP) replica, with an energy difference of 6.2 meV, in excellent agreement with the data of Olajos *et al.*

The PL of silver-doped silicon has been measured previously by Nazare *et al.* [5]; this spectrum shows the same A and B lines, but the LP interval is different.

The high-temperature data from figure 2 show two additional strong lines at, respectively, 811.6 and 806.1 meV. On increasing the temperature a detailed observation reveals that:

- The 806.1 meV band shows itself at a lower temperature, the 811.6 meV band appears later, but its intensity rises faster.
- The 806.1 meV band shifts to longer wavelengths.

From these observations, and the fact that the high-temperature lines are always seen together with the (low-temperature) A, B, and C lines, we suggest an explanation of these first-mentioned lines with a pseudodonor model [7], analogous to the description given by Thonke *et al.* for the C-line center in silicon [8].

Upon laser excitation, the neutral silver atom, Ag^0, $4d^{10}\ 5s^1$, will first capture a hole from the valence band, making the silver atom a positively charged ion, Ag^+. This ion can capture an electron from the conduction band, forming a bound exciton system of a pseudodonor character. Such a system can, for example, be visualized as a hole in a d shell and an electron in one of the outer orbitals, i.e., a $4d^9\ 5s^2$ or $4d^9\ 5s^1\ 5p^1$ electronic configuration; the extra 5s or 5p electron is much less tightly bound than the 4d hole. Formation of such configurations with a not completely filled d shell is indeed characteristic for transition metals. The p states of this electron can be calculated very well within the effective-mass approximation, but for the s states a large correction for the core potential should be applied.

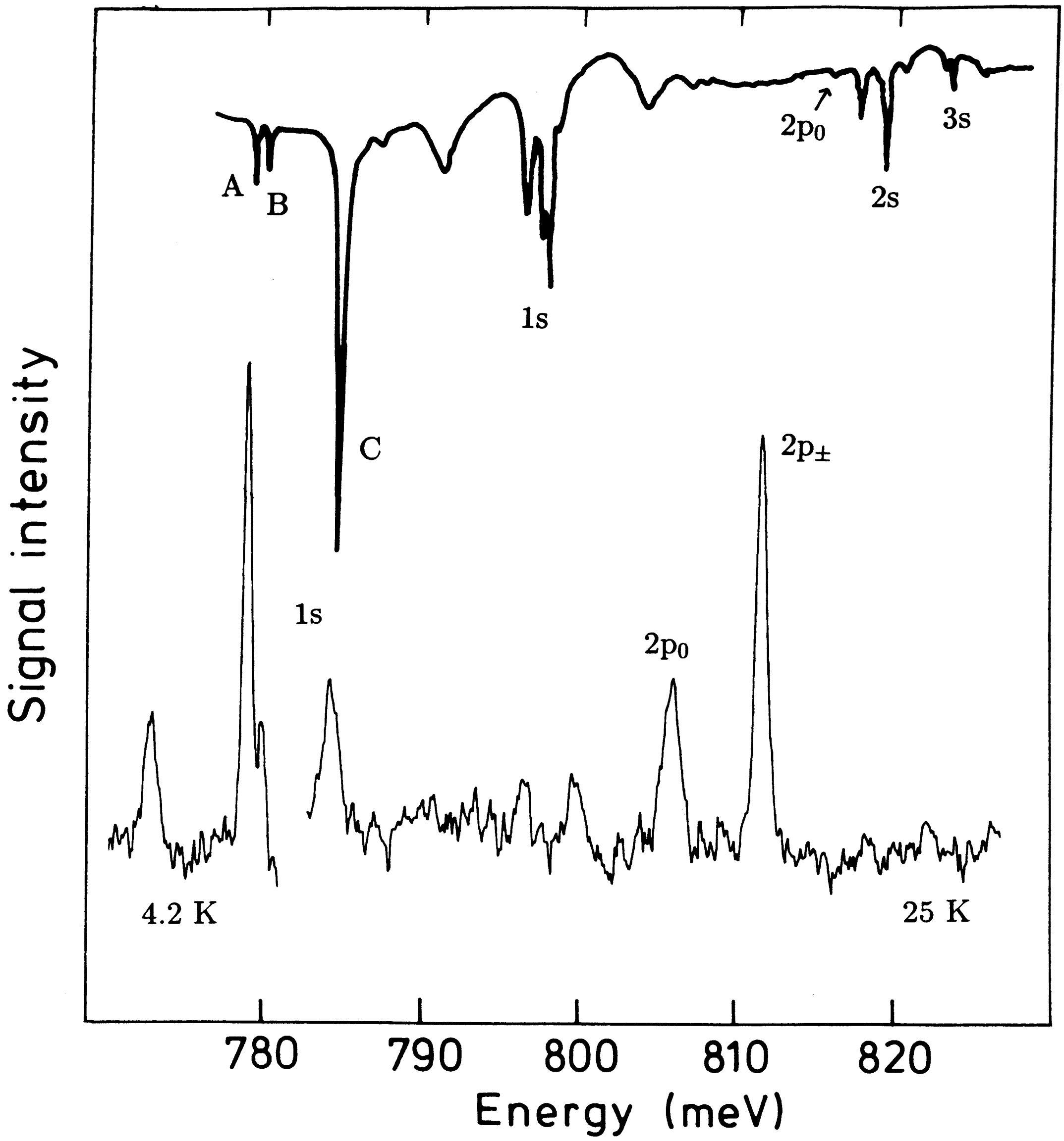

Figure 2: The 790-meV line at 4.2 and 25 K; the infra-red absorption spectrum of Olajos et al. [2] is also given (upper trace).

We suggest the line at 811.6 meV corresponds to the electron in the $2p_{\pm}$ state, whereas the 806.1 meV line is a superposition of the $2p_0$ state and a LP replica of the $2p_{\pm}$ line; a weak line at $\approx$ 800 meV should be a LP replica of the $2p_0$ line. The LP energy difference is then again 6.2 meV, which confirms our suggestion that these lines are due to the same silver center as observed by the low-temperature lines.

The energy level identification of this pseudodonor model is depicted in figure 2. If the $2p_{\pm}$ level lies at 811.6 meV, the end of the series would be at 818 meV. If the lowest energy level of the silver atom gives rise to the A line with an energy of 779 meV, the ionization energy of the extra electron is calculated at 39 meV. With an energy gap of silicon at this temperature of 1169 meV, we further calculate the binding energy of the hole as $\approx$ 351 meV. This value is in agreement with the DLTS determination, which yields for the donor level of silver E_v + 340 meV.

This pseudodonor interpretation is further confirmed by the high-temperature data as shown in figure 1: at higher temperatures a broad PL band appears just above $\approx$ 818 meV, which is interpreted as above-gap excitation.

It seems reasonable to suggest that upon laser excitation, a considerable number of silver centers will be transformed to this latter configuration; this requires, however, a large number of available holes and electrons. Such a transformation would be less probable in an infra-red absorption experiment.

One could also speculate about the microscopic origin of the 779-meV-PL band. We can make the following observations:

- It appears certain that the observed photoluminescence and the infra-red absorption measurements [2] pertain to the same center, which must then be a silver-containing defect. This is supported by the agreement with the DLTS data, and by corresponding LP values in all cases.
- If our interpretation as a transformation into a configuration with a deeply-bound hole in a 4d shell is correct, then it would require a (more or less isolated) silver *atom*. The defect is therefore most likely a single interstitial silver atom.

We therefore suggest the 779-meV band is due to isolated interstitial atoms, and corresponds with the EPR observation of the Si-NL42 center.

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