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INVESTIGATION OF DEFECT FORMATION PROCESSES IN SILICON WITH IRON IMPURITY

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Abstract. *The formation of defect centers in silicon doped with iron was studied. It is shown that a single deep level with an ionization energy* $E_V + 0.41$ *eV is associated with iron atoms in Si, and it is quickly annealed at low temperatures. The preliminary introduction of dysprosium and ytterbium impurities into the silicon volume leads to stabilization of the properties of the iron level in silicon was found.*
Keywords: *silicon, iron, dysprosium, ytterbium, deep level, annealing, stabilization.*

For the first time, deep levels (DL), which are formed by Fe in Si, were investigated in [1–2] from the temperature dependence of the Hall EMF and it was shown that Fe forms a donor level with an ionization energy $E_v + 0.4$ eV. This level is unstable, and at room temperature, the conversion of the $E_v + 0.4$ eV level to the donor $E_c - 0.55$ eV occurs. The authors of [2] from the study of the kinetics of the decomposition of the solid solution of Fe in Si showed that the solid solution Si - Fe is unstable (the electrical properties of Si<Fe> change even at room temperature). In [2–3], from electrical measurements and studies of the EPR spectra, it was assumed that this level exhibits acceptor properties after interaction with vacancies. As follows from the above, the results of published works devoted to the behavior of Fe in Si are contradictory.

The aim of this work was to study the processes of formation of defect centers in silicon doped with an iron impurity.

Using a complex of methods of capacitive spectroscopy (non-stationary capacitive deep-level spectroscopy (DLTS) and photocapacity (PC)), the effect of thermal treatments on the properties of deep centers created by Fe atoms was studied.

Silicon was doped with Fe as a diffusion method in the temperature range of $900 \div 1250^0$C for $0.5 \div 2$ h, followed by fast or slow cooling. For alloying, n-Si was used with an initial specific resistance from 1 to 300 Ohm.cm and p-Si from 1 to 300 Ohm.cm. After diffusion at T_d = 900-950^{0}C, the resistivity of n-Si and p-Si remained almost unchanged. In n-Si crystals at T> 1000^{0}C, the resistivity after diffusion of the Fe impurity decreased, and in p-Si, the value of ρ increased. The resistivity of the control samples that underwent a similar heat treatment remained almost unchanged. From the change in the value of ρ in Si after doping with Fe atoms, it can be concluded that Fe atoms introduce donor centers. The cooling rate of the samples after diffusion varied from 0.1^{0}C/s to 40-70^{0}C/s. Upon slow cooling after diffusion (0.1^{0}C/s), the concentration of photoactive impurity centers was somewhat lower (approximately by a factor of 3–5).

Diode structures were made from uncompensated crystals to measure the DLTS and PC spectra [4]. From the capacitance-voltage characteristics, the dependences $1/C^2 = f(V_{rev})$ are determined. These dependencies were linear in all studied diodes. The concentration of ionized centers in the space charge layer in n-Si diodes with T-ion impurities, as well as in p-Si with the Fe impurity, determined from the dependence $1/C^2 = f\ (V_{sample})$ at 300 K, agrees well with the concentration of small dopants in the original silicon.

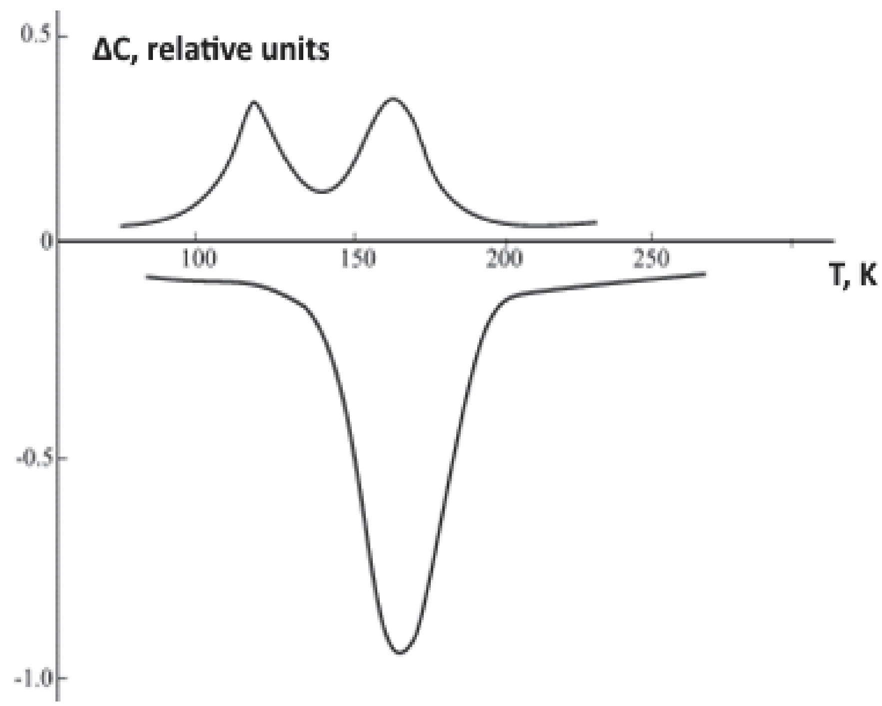

Fig. 1. Typical DLTS spectra of Si <Fe> samples

DLTS measurements in the initial silicon crystals showed that the concentration of deep level in them does not exceed 10^{11}cm^{-3}. After the diffusion introduction of iron into n-Si, the total concentration of ionized centers in the space charge layer does not change at 300 K and at 77 K in the dark. This indicates that iron forms only donor levels in silicon, and they are located in the lower half of the band gap (Fig. 1).

Measurements using capacitive spectroscopy have shown that in silicon doped with iron, three deep levels are formed with fixed ionization energies: two levels in the upper half of the band gap, E_c – 0.20 eV, E_c – 0.33 eV, with cross sections for the capture of charge carriers $\sigma_n = 4 \cdot 10^{-17}$cm^2 and $\sigma_n = 2 \cdot 10^{-15}$cm^2, respectively, and one deep level in the lower half of the forbidden zone E_v + 0.41 eV with charge carrier capture cross sections $\sigma_p = 2 \cdot 10^{-16}$ cm^2, respectively.

An analysis and comparison of the results with the control samples without Fe show that the deep level E_v + 0.41 eV is associated with iron atoms, and the levels E_c – 0.20 eV, E_c – 0.33 eV are probably heat treatment defects.

Measurements of the spectra of the PC and the induced PC (Fig. 2) showed that deep level formed by doping Si with iron is indeed in the lower half of the band gap: E_v + 0.41 eV with the hole capture cross section $\sigma \sim 10^{-14}$ cm^2.

The results of various low-temperature treatments at 100 ÷ 200°C showed that deep levels associated with iron atoms in silicon are unstable. Upon annealing at 150°C, the concentration of the E_v + 0.41 eV level decreases by a factor of 3-5.

We tried to stabilize the iron level by preliminary alloying with rare earth elements (REE) [5-6].

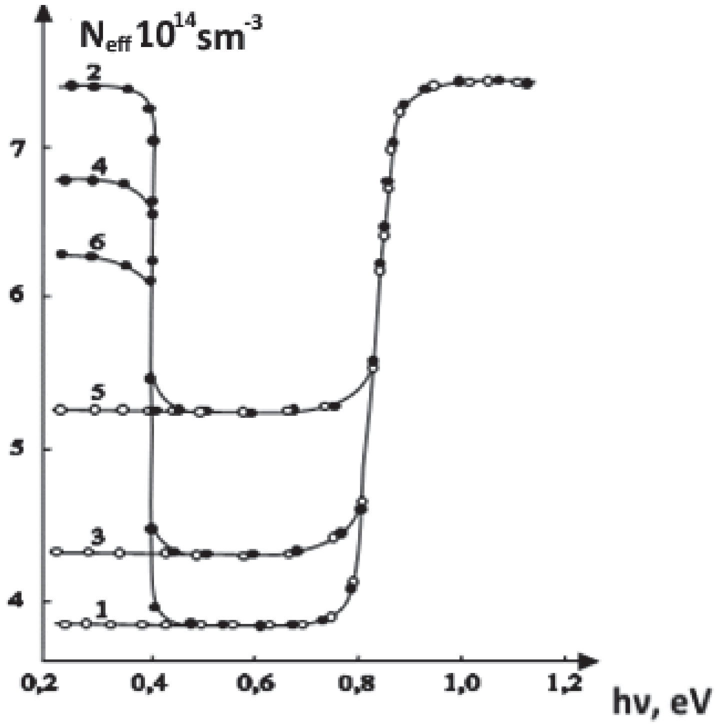

Fig. 2. Spectra of PC and induced PC of n-Si <Fe> samples after various low-temperature treatments

Measurements of the DLTS and PC spectra of the n-Si <Dy, Fe> and n-Si <Yb, Fe> samples showed that the preliminary introduction of dysprosium or ytterbium impurities into Si, followed by doping with iron leads to the stabilization of the E_v + 0.41 eV level, at 100 ÷ 200^0C it significantly slows down.

Thus, the results of the performed studies have shown that a single deep level with an ionization energy E_v + 0.41 eV is associated with iron atoms in Si, and it is rapidly annealed at low temperatures. The properties of the iron level in silicon can be stabilized by preliminary introduction of rare-earth impurities into the silicon volume.

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