Influence of Vacancy Defects on Compensation in Semi-Insulating VGF-GaAs

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Motivation

The carrier concentration and the resistivity in LEC (Liquid Encapsulated Czochralski)-GaAs optimized e.g. for ion-implantation processes can be described by a compensation model involving the intrinsic EL2 defect, the dominating extrinsic acceptor carbon, and residual impurities acting as shallow donors and acceptors.

The independent determination of intrinsic and extrinsic acceptor and donator concentrations and the agreement with the compensation model is the basis for reliable production of semi-insulating GaAs-substrates.

The content of electrically active defects in GaAs strongly depends on the impurity concentration of the basis materials as well as on the growth technology.

Comparing static electrical properties as a function of carbon content a slight deviation from typical values of state-of-the-art LEC material is observed for a group of samples from VGF-grown ingots.

Results from chemical analysis by AES (atom emission spectroscopy) and GDMS (glow-discharge mass spectroscopy) show, that this deviation cannot be due to additional extrinsic defects.

Compensation Model

- formalism according to [1], considered defects cf. Tab. 1
- In contrast to LEC-grown GaAs, an additional acceptor is required to explain the compensation in VGF (Vertical Gradient Freeze)-GaAs.
- concentration of missing acceptor was calculated for the VGF-samples

defect	electrical property	defect parameters	quantitative measurement technique	concentration used for modelling [cm^{-3}]
EL2	deep double donor	$E_a^{0/+} = E_C - 0.69$eV $E_a^{+/++} = E_C - 0.9$eV $g_0 = 1$ $g_1 = 2$ $g_2 = 1$	IR-Absorption	3.2×10^{16}
C_{As}	shallow acceptor	$E_a^{-/0} = E_V + 0.027$eV $g_0 = 4$ $g_1 = 1$	local vibrational mode spectroscopy	variable (1×10^{14} - 1×10^{16})
oc-O_{As}	middle deep negative U center	$E_a^{-/0} = E_C - 0.59$eV $E_a^{0/+} = E_C - 0.14$eV $g_0 = 1$ $g_1 = 2$ $g_2 = 1$	local vibrational mode spectroscopy	1×10^{14}
Σ (Si_{Ga}, S_{As}, Se_{As}, ...)	shallow donors	$E_a^{-/0} \approx E_C$ - 0.005eV $g_0 = 1$ $g_1 = 2$	AES, GDMS	1×10^{14}
Σ (Zn_{Ga}, Mg_{Ga}, Ge_{As}, ...)	shallow acceptors	$E_a^{-/0} \approx E_C$ - 0.03eV $g_0 = 4$ $g_1 = 1$	AES, GDMS	4×10^{14}

Tab. 1: **defects and defect parameters used for calculation of carrier concentration in S.I. GaAs samples**

neutrality condition:

$$n = p + \sum_k \sum_{l=0}^{l_{Dk}+l_{Ak}} \left(l_{Dk} - l\right) n_{kl}$$

$$n_{kl} = \frac{1}{1 + \sum_{l'=0,l'\neq l}^{l_{Dk}+l_{Ak}} \frac{g_{kl'}}{g_{kl}} e^{-\frac{(\varepsilon_{kl'} - l'E_F) - (\varepsilon_{kl} - lE_F)}{k_B T}}}$$

g_{kl} : degeneracy factor of l^{th} state of k^{th} defect
ε_{kl} : energy of l^{th} state of k^{th} defect relative to valence band maximum
l_{Dk} : no. of donor states of k^{th} defect
l_{Ak} : no. of acceptor states of k^{th} defect

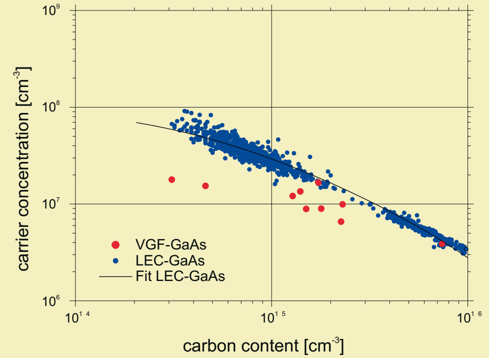

Fig. 1 **Carrier concentration vs. carbon content for S.I. GaAs. Devation of VGF sample data from typical LEC data indicates presence of additional acceptor(s).**

Experimental

- Positron lifetime spectroscopy was done with a standard fast-fast spectrometer (time resolution 250 ps).
- The momentum distribution was observed with a Doppler coincidence setup consisting of two Ge-detectors (resolution of 1.03 keV) [2].

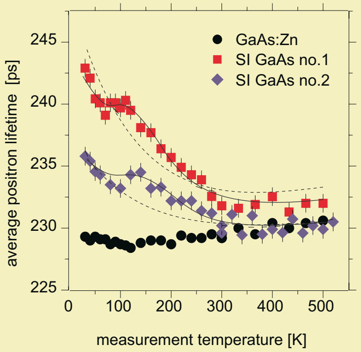

Fig. 2 **Average positron lifetime as a function of the measurement temperature in SI-GaAs compared to a GaAs:Zn reference. Lines are fits to the data assuming positron trapping at neagtive vacancies and negative ions (solid lines) or at negative vacancies only (dashed lines).**

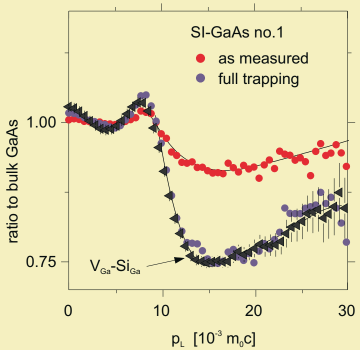

Fig. 3 **Momentum distribution in SI-GaAs (sample no. 1 (*Fig. 2*), measured at 30K) compared to that of the V_{Ga}-Si_{Ga} complex in highly Si-doped GaAs. Lines are guide to the eye only.**

Positron Results

- lifetime measurements: τ_b ~229 ps @ 300 K [3]
  negatively charged monovacancy (τ_v ~260-270 ps)
- measurement of momentum distribution ➔ trapping in Ga-vacancy related defects (V_{Ga}, V_{Ga}-X_{Ga}) [4]
- fitting of temperature dependent trapping model [5]: negatively charged vacancies (E_b = 50 meV, $T_{r\text{-}V} \sim 10^{11}$ s^{-1} [3, 5])
  shallow positron trap (negative ions, E_b = 50 meV)
  fit parameter: trapping rates $\kappa_v(T)$, $\kappa_{st}(T)$
- In order to determine absolute defect concentrations C, trapping coefficients μ are necessary. ($\kappa = \mu_{20} (T/20K)^{-1/2}$ C [6])

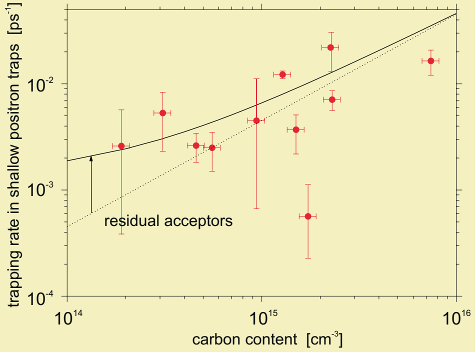

Fig. 4: **Trapping rate at shallow positron traps vs. carbon content. Solid line represents proportionality of trapping rate to net acceptor concentration (C_{As}^- + 4×10^{14} cm^{-3} residual acceptors)**

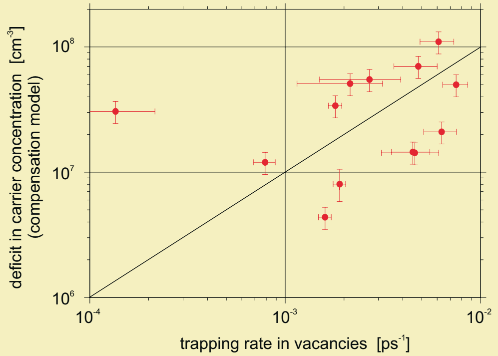

Fig. 5: **Difference of carrier concentration between typical LEC and VGF samples of the same carbon content as a function of positron trapping rate in vacancies.**

Correlations and trapping coefficients

- Trapping rate for positron trapping in shallow traps correlates very well with the net acceptor concentration (C_{As}^- + 4×10^{14} cm^{-3} residual acceptors).
- μ_{st} @ 20K = $(2.0\pm1.0)\times10^{17}$ s^{-1}
- For VGF-samples trapping rate for positron trapping in gallium vacancies is proportional to the deficit in carrier concentration derived from compensation model.
- assuming V_{Ga}^{3-} : μ_v @ 20K = $(1.5\pm1.0)\times10^{16}$ s^{-1}
- assuming $(V_{Ga}$-$X_{Ga})^-$: μ_v @ 20K = $(4.5\pm2.5)\times10^{16}$ s^{-1}

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Conclusion

- The slight deviation of the static electrical properties of VGF GaAs from typical state-of-the-art LEC material is due to a additional acceptor which was identified as a V_{Ga}-related defect. A proportionality of the expected acceptor concentration and the vacancy concentration was observed.
- Assuming different charge states of the V_{Ga}-related defect the trapping coefficient can be independently estimated. The obtained values are consistent with literature [3, 7]
- The correlation between trapping rate for positron trapping in shallow traps and net acceptor concentration leads to a trapping coefficient of $(2.0\pm1.0)\times10^{17}$ s^{-1} @ 20K. This is one of the first independently obtained values for shallow positron traps in GaAs.