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J. Phys.: Condens. Matter 14 (2002) 7963-7971

# Interactions of point defects with dislocations in n-type silicon-doped GaAs

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Received 15 May 2002, in final form 18 June 2002 Published 15 August 2002 Online at stacks.iop.org/JPhysCM/14/7963

### Abstract

Raman scattering and cathodoluminescence experiments have been performed to investigate the effect of dislocations on the spatial distribution of point defects and on the free electron concentration in n-type GaAs:Si. An experimentally extended increase of the free electron and  $(Si_{Ga}V_{Ga})^{2-}$  complex concentrations from the matrix to the dislocation is explained as resulting from the formation of arsenic precipitates around the dislocation by means of computer simulations based on a diffusion-aggregation model.

#### 1. Introduction

With the development of semiconductor techniques, the III-V family of compound semiconductors such as GaAs have been widely applied in high-frequency and optoelectrical devices. Since point and extended defects are inevitably created during fabrication of semiconductor materials, it is thus essential to understand how the defects affect their electrical and optical properties. A dislocation, among the extended defects, is well known to act as a sink to capture dopants, forming a Cottrell atmosphere and so leading to an inhomogeneous distribution of the electrical and optical properties of the materials. Although extensive investigations based mainly on experimental observations have been performed on this area, there are still some issues that need clarifying further. For example, the reduction of the concentration of  $Si_{As}^{-}$  (Te<sub>As</sub><sup>+</sup>) acting as acceptors (donors) was recently suggested as explaining the significant increase (decrease) of the free electron concentration (FEC) from the matrix to the dislocations in n-type GaAs:Si (Te) [1]. However, the explanation is suspect, especially for n-type GaAs:Si, since the Si<sub>As</sub> concentration in n-type GaAs:Si is much lower compared to the  $Si_{Ga}^+$  concentration, so the reduction of the  $Si_{As}^-$  concentration cannot drastically change

0953-8984/02/347963+09\$30.00 © 2002 IOP Publishing Ltd Printed in the UK

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the spatial distribution of the FEC. In fact, the deduction mentioned above conflicts with our recent experimental observations on n-type GaAs:S, where sulphur, like Te, occupies the arsenic sites while the FEC increases from the matrix to the dislocation, contrary to the case for GaAs:Te. On the other hand, the defect complexes have long attracted attention due to their technological and scientific interest. Researchers have found that a donor at an arsenic lattice site such as  $Te_{As}^+$  in GaAs:Te and  $S_{As}^+$  in GaAs:S or at a gallium site such as  $Si_{Ga}^+$  in n-type GaAs:Si can combine with a gallium vacancy to form a nearest-neighbour or a second-nearestneighbour complex [2]. However, the effects of dislocations on the complexes have hardly been explored. In particular, although arsenic precipitates were observed to be commonly formed at the dislocations in GaAs doped with Cr, O, Si and Zn [1, 3], it is still unknown to what extent they can influence the spatial distribution of point defects and of the FEC.

Here, we focus on several issues with the aim of providing some understanding of the spatial distribution of the point defects and of the FEC due to the existence of dislocations. To this end, we use Raman scattering and cathodoluminescence (CL) to investigate the interactions of point defects and dopants with the as-grown dislocations in n-type GaAs:Si, combining these with computer simulations in which microscopic diffusion–aggregation processes are carefully taken into account.

#### 2. Experiment

The samples of n-type Si-doped GaAs(100) with about  $1.0 \times 10^{18}$  silicon atoms cm<sup>-3</sup> were grown by the vertical gradient freezing (VGF) technique and were then cleaned by mechanochemical polishing. In order to expose the as-grown dislocations at the sample surface to Raman scattering, the samples were etched by a dilute sirtle-like photoetching (DSL) procedure [4]. After that, they were transferred to Raman and scanning electron microscope (SEM) CL microscopes for acquisition of the relevant information.

The 632.8 nm line of a He–Ne laser with a power of 25 mW was used for the Raman scattering investigation. The laser beam was focused on the sample with a spot size of 1  $\mu$ m. The scattered light was collected and analysed by a Dilor Labram microscope with a CCD detector. The spectral resolution is better than 0.1 cm<sup>-1</sup> and the spatial resolution is below 1  $\mu$ m. All spectra were recorded in the backscattering geometry at room temperature.

The samples were further observed in the secondary-electron (SE) and CL modes in a JSM 6400 SEM equipped with an Oxford monochromatic CL system at a temperature of 75 K. A 20 keV electron beam was selected to excite the samples. Photomultiplier and Ge detectors were used to process the corresponding CL images and spectra.

#### 3. Diffusion model

To improve the understanding of the interactions of point defects with the dislocations, a microscopic diffusion–aggregation model was constructed. As suggested by You *et al* [5], this model supposes that silicon diffuses via Ga vacancies. The negative triply charged state of a Ga vacancy assumed for  $V_{Ga}^{3-}$  was found to be the main Ga vacancy at all doping levels [6]. The diffusion mechanism has been confirmed theoretically [7]. It is known that nearly all Si atoms occupy only Ga sites when the silicon concentration is below  $5 \times 10^{18}$  cm<sup>-3</sup>, as in the present GaAs:Si samples. So the conversion of the Si<sub>Ga</sub> species into Si<sub>As</sub> species is neglected in our simulations. Since the (Si<sub>Ga</sub>V<sub>Ga</sub>)<sup>2-</sup> complexes have been observed in the present CL spectra, their effect must be incorporated into the diffusion–aggregation model. A (Si<sub>Ga</sub>V<sub>Ga</sub>)<sup>2-</sup>

complex is formed by the reaction

$$\mathrm{Si}_{\mathrm{Ga}}^{+} + \mathrm{V}_{\mathrm{Ga}}^{3-} \rightleftharpoons (\mathrm{Si}_{\mathrm{Ga}} \mathrm{V}_{\mathrm{Ga}})^{2-}.$$
 (1)

In order to process the information on the spatial distribution of point defects, a set of partial differential equations including the diffusion–aggregation processes for  $Si_{Ga}^{+}$ ,  $V_{Ga}^{3-}$  and  $(Si_{Ga}V_{Ga})^{2-}$  were solved numerically:

$$K^{+}C_{\mathrm{Si}_{\mathrm{fa}}^{\mathrm{eq}}}^{\mathrm{eq}}C_{\mathrm{V}_{\mathrm{fa}}^{\mathrm{a}-}}^{\mathrm{eq}} = K^{-}C_{(\mathrm{Si}_{\mathrm{fa}}\mathrm{V}_{\mathrm{Ga}})^{2-}}^{\mathrm{eq}}$$
(2)

$$\frac{\partial C_{(\mathrm{Si}_{\mathrm{Ga}}\mathrm{V}_{\mathrm{Ga}})^{2^{-}}}}{\partial t} = K^{+}C_{\mathrm{Si}_{\mathrm{Ga}}^{+}}C_{\mathrm{V}_{\mathrm{Ga}}^{3^{-}}} - K^{-}C_{(\mathrm{Si}_{\mathrm{Ga}}\mathrm{V}_{\mathrm{Ga}})^{2^{-}}}$$
(3)

$$\frac{\partial C_{\mathrm{Si}_{\mathrm{Ga}}^{+}}}{\partial t} = \frac{\partial}{\partial r} \left[ D_{\mathrm{Si}_{\mathrm{Ga}}^{+}} \left( \frac{\partial C_{\mathrm{Si}_{\mathrm{Ga}}^{+}}}{\partial r} + \frac{C_{\mathrm{Si}_{\mathrm{Ga}}^{+}}}{n} \frac{\partial n}{\partial r} + \frac{C_{\mathrm{Si}_{\mathrm{Ga}}^{+}}}{k_{B}T} \frac{\partial \phi_{\mathrm{Si}_{\mathrm{Ga}}^{+}}}{\partial r} \right) \right] - \frac{\partial C_{(\mathrm{Si}_{\mathrm{Ga}}\mathrm{V}_{\mathrm{Ga}})^{2^{-}}}}{\partial t} + \omega_{1}$$
(4)

$$\frac{\partial C_{\mathrm{V}_{\mathrm{Ga}}^{3-}}}{\partial t} = \frac{\partial}{\partial r} \left[ D_{\mathrm{V}_{\mathrm{Ga}}^{3-}}} \left( \frac{\partial C_{\mathrm{V}_{\mathrm{Ga}}^{3-}}}{\partial r} - 3 \frac{C_{\mathrm{V}_{\mathrm{Ga}}^{3-}}}{n} \frac{\partial n}{\partial r} + \frac{C_{\mathrm{V}_{\mathrm{Ga}}^{3-}}}{k_B T} \frac{\partial \phi_{\mathrm{V}_{\mathrm{Ga}}^{3-}}}{\partial r} \right) \right] - \frac{\partial C_{(\mathrm{Si}_{\mathrm{Ga}}\mathrm{V}_{\mathrm{Ga}})^{2-}}}{\partial t} + \omega_2 \tag{5}$$

where *t* is the diffusion–aggregation time, *r* the distance from the dislocation core,  $k_B$  the Boltzmann constant and *T* the temperature in kelvins;  $C_{Si_{Ga}^+}$ ,  $C_{V_{Ga}^{3-}}$  and  $C_{(Si_{Ga}V_{Ga})^{2-}}$  are the concentrations of Si<sub>Ga</sub><sup>+</sup> donors and of V<sub>Ga</sub><sup>3-</sup> and (Si<sub>Ga</sub>V<sub>Ga</sub>)<sup>2-</sup> acceptors,  $D_{Si_{Ga}^+}$  and  $D_{V_{Ga}^{3-}}$  are the diffusion coefficients of Si<sub>Ga</sub><sup>+</sup> and V<sub>Ga</sub><sup>3-</sup>, respectively; *n* is the FEC;  $\omega_1$  and  $\omega_2$  are related to the effects of other possible factors such as the formation of precipitates at the dislocation;  $\phi$  is the purely radial interaction potential between a Si atom ( $\phi_{Si_{Ga}^+}$ ) or a Ga vacancy ( $\phi_{V_{Ga}^{3-}}$ ) and a dislocation and is taken in the framework of elastic theory simply as  $\phi = A/r$  with the constant *A* equal to  $3.5 \times 10^{-5}$  eV  $\mu$ m for  $\phi_{Si_{Ga}^+}$  and  $0.4.6 \times 10^{-7}$  eV  $\mu$ m for  $\phi_{V_{Ga}^3-}$  [8]. The Fermi-level effect is actually considered by explicitly introducing the FEC in equations (4) and (5) according to [6]. Under the assumption that the reaction in equation (1) is locally in equilibrium at the initial time, the equilibrium concentrations  $C_{Si_{Ga}^+}^{eq}$ ,  $C_{V_{Ga}^3-}^{eq}$  and  $C_{(Si_{Ga}V_{Ga})^{2-}}^{eq}$  are the reaction constants for the forward and backward reactions of equation (1) and  $K^+$  is given after the theory of Waite [9]:

$$K^{+} = 4\pi r_{c} (D_{\mathrm{Si}_{\mathrm{Ga}}^{+}} + D_{\mathrm{V}_{\mathrm{Ga}}^{3-}}).$$
(6)

Here  $r_c$  is the distance between Si<sup>+</sup><sub>Ga</sub> and V<sup>3-</sup><sub>Ga</sub> and was taken as  $\sqrt{2}/2a$  (*a* is the lattice constant of GaAs);  $D_{\text{Si}_{\text{Ga}}^+}$  and  $D_{\text{V}_{\text{Ga}}^{3-}}$  are functions of the FEC:

$$D_{\mathrm{Si}_{\mathrm{Ga}}^{+}}(n) = D_{\mathrm{Si}_{\mathrm{Ga}}^{+}}(n_{i}) \left(\frac{n}{n_{i}}\right)^{3}$$

$$\tag{7}$$

$$D_{V_{Ga}^{3-}}(n) = D_{V_{Ga}^{3-}}(n_i) \left(\frac{n}{n_i}\right)^3.$$
(8)

The FEC *n* is dependent on  $C_{\text{Si}_{\text{Ga}}^+}$ ,  $C_{\text{V}_{\text{Ga}}^{3-}}$  and  $C_{(\text{Si}_{\text{Ga}}\text{V}_{\text{Ga}})^{2-}}$  as well as on the intrinsic electron concentration  $n_i$ :

$$n = \frac{1}{2} \left[ (C_{\mathrm{Si}_{\mathrm{Ga}}^{+}} - 3C_{\mathrm{V}_{\mathrm{Ga}}^{3-}} - 2C_{(\mathrm{Si}_{\mathrm{Ga}}\mathrm{V}_{\mathrm{Ga}})^{2-}}) + \sqrt{(C_{\mathrm{Si}_{\mathrm{Ga}}^{+}} - 3C_{\mathrm{V}_{\mathrm{Ga}}^{3-}} - 2C_{(\mathrm{Si}_{\mathrm{Ga}}\mathrm{V}_{\mathrm{Ga}})^{2-}})^{2} + 4n_{i}^{2}} \right]. \tag{9}$$

Although the diffusion of silicon is controlled directly by Ga vacancies, the effect of interstitial arsenic is carefully considered in the present simulations in the following reaction:

$$\mathbf{V}_{\mathrm{Ga}} + \mathbf{I}_{\mathrm{As}} \rightleftharpoons \mathrm{As}_{\mathrm{Ga}}.\tag{10}$$

This reaction was suggested to explain why an increase in EL2 concentration related to the arsenic antisite ( $As_{Ga}$ ) is accompanied by lessening of the formation of arsenic precipitates [10].

The formation of arsenic precipitates reduces the concentration of  $I_{As}$ , so the reaction in equation (10) proceeds from the right to the left, causing an increase in  $C_{V_{Ga}^{3-}}$ . In order to characterize this effect,  $\omega_2$  is estimated simply as

$$\omega_2 = \alpha \Big( C_{\mathrm{V}_{\mathrm{Ga}}^{3-}} - C_{\mathrm{V}_{\mathrm{Ga}}^{3-}}^{\mathrm{eq}} \Big).$$
(11)

Here  $\alpha$  is an adjustable parameter used to determine the rate of formation of precipitates and a larger  $\omega_2$  means a higher formation rate. Since the actual solubility of Si in GaAs is extremely large (e.g. about  $1.0 \times 10^{20}$  cm<sup>-3</sup> at 950 °C) and no silicon precipitate is hence expected in the GaAs:Si samples investigated according to the classical nucleation theory [11],  $\omega_1$  is set to zero.

#### 4. Results and discussion

In figure 1(a), a high-intensity TO-like mode can be observed at about 263 cm<sup>-1</sup>. The fact that the weak LO mode contrasts with the strong TO-like peak seems contrary to the general selection rule, according to which only the LO mode is Raman active for the GaAs(100) surface. The x-ray diffraction indicates that the surface of GaAs is indeed (100). To confirm these measurements, another Raman scattering study on semi-insulating GaAs(100) has been made to show the good agreement with the selection rule, i.e. that only the LO phonon can be observed in the backscattering geometry. The appearance of the TO-like peak can thus be attributed to a doping effect, in which the LO mode is split into two submodes: the lowfrequency branch  $L^-$  and the high-frequency one  $L^+$ , introduced by phonon–plasma coupling. Therefore, the TO-like peak is contributed mainly by the  $L^-$  mode. Figure 1(a) shows further that the  $L^+$  peak at the dislocation is at a higher frequency position than for the matrix, which implies a higher FEC. Calculating the ratio of the integrated intensity of the  $L^-$  peak to that of the LO peak [12] or the position of the  $L^+$  peak [13] as shown in figure 1(a), the FEC can be obtained as  $9.5 \times 10^{17}$  cm<sup>-3</sup> in the matrix and increases from the matrix to the dislocation (figure 1(b)). Additionally, the inset of figure 1(a) displays a Raman peak at the spectral position of 257 cm<sup>-1</sup>, occasionally detected around the dislocations, which is assigned to LO mode of hexagonal arsenic precipitates [1].

Detailed examination of the LO peak in figure 1(a) indicates that this peak shifts down by  $1.5 \text{ cm}^{-1}$  in the matrix and  $2.5 \text{ cm}^{-1}$  at the dislocation in GaAs:Si compared to that for semiinsulating GaAs. Although the feature has been observed for p-type GaAs (e.g. GaAs:Zn [14] and GaAs:Be [15]), it was usually overlooked in the case of n-type GaAs. It is generally certain that a negative frequency shift implies the existence of tensile strain. If a conversion factor of 0.0034 cm from the Raman shift to the strain is applied [16], strains of 0.51% in the matrix and of 0.80% at the dislocation are achieved. Although early experiments have found the lattice distance of GaAs to increase linearly with silicon concentration at a rate of  $2.0 \times 10^{24}$  nm cm<sup>-3</sup> when the FEC is below  $2.0 \times 10^{18}$  cm<sup>-3</sup> [17], a tensile strain based on this relationship is too small to explain the pronounced shift of the LO peak. There are thus other factors responsible for the negative frequency shift. It is well known that only single phonons near the centre of the Brillouin zone (wavevector  $q \approx 0$ ) can contribute to the Raman spectra in an infinite crystal because the momentum of phonons and photons must be conserved, but phonons can be confined in defects in a real crystal, which results in non-conserved momenta and thus allows phonons with  $q \neq 0$  to contribute to the Raman spectra [18]. As a result, the line shape of the Raman spectra may be broadened and asymmetric. Considering this, a so-called spatial correlation model was constructed [18]. According to this model, LO peaks are fitted and presented in figure 1(c), which exhibits a reasonable agreement with experimental results. Therefore, the negative frequency shift probably originates from an enhanced wavevectornon-conserving scattering induced by Si dopants, implying the aggregation of Si around the dislocation [14].



**Figure 1.** (a) Raman spectra of the matrix of semi-insulating GaAs(100), of GaAs(100):Si and for around the dislocation of GaAs:Si; inset: a typical spectrum detected from the dislocation, exhibiting the arsenic precipitates formed; (b) a mapping of the spatial distribution of the FEC from the matrix (M:  $(9.70\pm0.50) \times 10^{17} \text{ cm}^{-3}$ ) to the dislocation (D:  $(1.15\pm0.35) \times 10^{18} \text{ cm}^{-3}$ ); (c) the fitting of the LO peak (curve) by the Raman correlation model. For comparison, experimental data are also plotted (curve + symbols). The two peaks obtained by fitting and from experiment on the right are related to semi-insulating GaAs (SI), the peaks in the middle to the matrix (M) and the ones on the left to the dislocation (D) in GaAs:Si.

After performing our Raman scattering study, we turn next to CL measurements. Panchromatic CL images over a wavelength range from 400 to 900 nm were acquired by a photomultiplier and one of them is displayed in figure 2(a). The image exhibits dark dots corresponding to the dislocations, as non-radiative recombination centres, contrasting with bright surroundings. Similarly, figure 2(b) displays another panchromatic CL image for the same spatial region obtained by a Ge detector, whose detection range is from 900 to 1400 nm. In spite of a weaker contrast between the dislocation and the matrix, figure 2(b) shows the same trend for the CL intensity as figure 2(a), i.e. the total CL intensity decreases from the matrix to the dislocation. In fact, as indicated in figures 2(c) and (d), the CL images in figures 2(a) and (b) are connected to near-band-edge (NBE),  $B_{As}^-$  acceptor-related and  $(Si_{Ga}V_{Ga})^{2-}$  complex-related emissions, respectively. The NBE band has shifted up from 820 nm (1.51 eV) for semi-insulating GaAs at 75 K to 840 nm for GaAs:Si due to the doping effect (figure 2(c)).  $B_{As}$  is contributed by the encapsulant (boron oxide) used for growing the GaAs samples.

In addition to the NBE transition peak, two more typical peaks at 930 nm (1.33 eV) and at 1080 nm (1.15 eV) have been measured in CL spectra (figure 2(d)). The 1.15 eV band is identified as a transition within the Si<sub>Ga</sub> donor–Ga vacancy complex [2] while the 1.33 eV band is due to the recombination from near the conduction band to the acceptor  $B_{As}^-$  state [19]. It is well known that CL intensity is proportional to the concentration of the electron–hole pairs available for recombination times the ratio of their effective lifetime  $\tau_e$  to the radiative lifetime  $\tau_{rad}$ . And  $\tau_e$  is given by

$$\frac{1}{\tau_e} = \frac{1}{\tau_{rad}} + \frac{1}{\tau_{nonrad}}.$$
(12)

Equation (12) states that  $\tau_e/\tau_{rad}$  is no larger than one because of the competition from nonradiative recombination centres such as dislocations. Therefore, the difference in experimental CL intensities of  $(Si_{Ga}V_{Ga})^{2-}$  complexes cannot indicate whether the complex concentration increases or not. If the concentration of the electron–hole pairs responsible for the NBE band is supposed to be the same over the whole region and  $\tau_e/\tau_{rad}$  to remain constant for different emission bands at the same position, the intensities of the two (1.33 and 1.15 eV) bands are normalized simply to the NBE band so as to eliminate the passive effect of a dislocation as a non-radiative centre when evaluating the spatial variation of the complex concentrations. Figure 2(d) shows that the normalized CL intensity of the two bands increases from the matrix to the dislocation, implying an important enhancement of  $B_{As}$  and the complexes around the dislocations.

In order to explain why the free electron and  $(Si_{Ga}V_{Ga})^{2-}$  complex concentrations increase from the matrix to the dislocation, computer simulations based on a diffusion–aggregation model as described in equations (2)–(8) were performed. At the initial time (t = 0), the silicon dopants were distributed homogeneously from the matrix to the dislocation and the Si concentration was selected as  $1.0 \times 10^{18}$  cm<sup>-3</sup> so that the FEC in the matrix is nearly the same as the experimental one. The simulations were made at 950 °C, so the corresponding  $C_{V_{Ga}^{3-}}$  and  $C_{(Si_{Ga}V_{Ga})^{2-}}$  were respectively  $1.50 \times 10^{16}$  and  $1.20 \times 10^{16}$  cm<sup>-3</sup> at t = 0 according to [7]. The simulations show that  $C_{Si_{Ga}^+}$ ,  $C_{V_{Ga}^{3-}}$  and  $C_{(Si_{Ga}V_{Ga})^{2-}}$ , if no precipitate is formed ( $\alpha = 0$ ), increase from the matrix to the dislocation with a short-range increasing region, i.e., only about  $0.05 \ \mu$ m (figure 3). Due to the aggregation around the dislocation,  $C_{Si_{Ga}^+/C_0}$  in the matrix must actually be a little below 1 to conserve the total number of  $Si_{Ga}^+$  donors in the whole region. In particular, in addition to the interaction between a Ga vacancy and a dislocation assumed in the diffusion–aggregation process (see equation (5)), the Fermi-level effect under consideration enhances the aggregation of  $V_{Ga}^{3-}$  and  $(Si_{Ga}V_{Ga})^{2-}$  complexes around the dislocation. In fact, an increase of the silicon concentration causes a higher Fermi level and thus reduces the formation



**Figure 2.** (a) A panchromatic CL image detected by a photomultiplier whose effective detection range is from 400 to 900 nm; the image comes mainly from near-band-edge emission (see (c)); (b) a panchromatic CL image detected by a Ge detector whose effective detection range is from 900 to 1400 nm; the image comes mainly from  $(B_{As})$  and  $(Si_{Ga}V_{Ga})^{2-}$  transitions (see (d)); (c) and (d) CL spectra of GaAs(100) at 75 K taken from points 1–3 marked in (a).

energies of the Ga vacancy and the  $(Si_{Ga}V_{Ga})^{2-}$  complex [7], increasing their concentrations. As a competition of the quantities of  $Si_{Ga}^+$  donors with that of  $V_{Ga}^{3-}$  and  $(Si_{Ga}V_{Ga})^{2-}$  acceptors, the FEC also becomes higher near the dislocation. However, the simulated increasing region of about 0.05  $\mu$ m is too small to match the experimental results from the Raman scattering study (see figure 1(b)), which show the region to be about 10  $\mu$ m beyond the dislocation.



**Figure 3.** (a) The simulated spatial distribution of  $Si_{Ga}^+$  and (b) the simulated spatial distributions of  $V_{Ga}^{3-}$  and  $(Si_{Ga}V_{Ga})^{2-}$  after 4 h at 950 °C (C<sub>0</sub> is the respective equilibrium concentration at the initial time); the corresponding distribution of the FEC is shown in the inset of (a). *r* is the distance from the dislocation.  $\alpha$  is in units of 1 s<sup>-1</sup>.

With some arsenic precipitates formed around the dislocation ( $\alpha = 1$  and 5), the increasing regions of  $C_{\text{Si}_{Ga}^{-}}$ ,  $C_{\text{V}_{Ga}^{-}}$  and  $C_{(\text{Si}_{Ga}\text{V}_{Ga})^{2^{-}}}$  as well as of the FEC are extended significantly up to 10  $\mu$ m or so. Comparison of the three cases with different values of  $\alpha$  indicates that the higher velocity of forming arsenic precipitates reduces further the number of Si\_{Ga}^{+} donors but increases those of  $C_{\text{V}_{Ga}^{-}}$  and  $C_{(\text{Si}_{Ga}\text{V}_{Ga})^{2^{-}}}$ , so the free electron concentration decreases with increasing  $\alpha$  at the same distance from the dislocation. In fact, the FEC is determined mainly by Si\_{Ga}^{+}, so it shows a similar trend to Si\_{Ga}^{+} since the numbers of  $\text{V}_{Ga}^{-}$  and  $(\text{Si}_{Ga}\text{V}_{Ga})^{2^{-}}$  are far lower than that of Si\_{Ga}^{+}. Experimentally, Raman scattering (figure 1(b)) and CL measurements (figures 2(b) and (c)) show that the free electron or (Si\_{Ga}\text{V}\_{Ga})^{2^{-}} complex concentration increases from the dislocation and, particularly, that the increasing region is broad, i.e. about 10  $\mu$ m from the dislocation outwards, comparable to the findings of the simulations with  $\alpha = 5$ . Therefore, direct comparison of computer simulations with Raman scattering and CL measurements indicates that the formation of arsenic precipitates is critical for spatial redistribution of the FEC and of (Si\_{Ga}^{-}\text{V}\_{Ga})^{2^{-}} complexes.

## 5. Conclusions

In summary, we have investigated the interactions of point defects with dislocations in the case of n-type Si-doped GaAs(100) by means of Raman scattering and CL investigations, combined with computer simulations based on a microscopic diffusion–aggregation model. The studies elucidate that the interactions induce silicon dopants, gallium vacancies and  $(Si_{Ga}V_{Ga})^{2-}$  complexes to diffuse to and to aggregate along the dislocations. Computer simulations reveal that the experimentally extended increasing region of the free electron and  $(Si_{Ga}V_{Ga})^{2-}$  concentrations originates from the formation of arsenic precipitates around the dislocation.

#### Acknowledgments

The authors thank Mr H Mähl for valuable technical support. This work was financed by the Kultusministerium Sachsen-Anhalt.

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