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LETTER TO THE EDITOR

Comparative models for diffusion of Be in InGaAs/InP heterostructures

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Abstract
A systematic study of Be diffusion from a Be-doped (3×10^{19} cm^{-3}) $In_{0.53}Ga_{0.47}As$ epilayer sandwiched between undoped InP epilayers was carried out. Using the boundary conditions and the segregation phenomena at InGaAs/InP interfaces, and taking into account built-in electric field, Fermi-level and bulk self-interstitial generation/annihilation effects, the concentration profiles of Be in the InGaAs/InP heterostructure have been simulated according to two 'kick-out' models. Comparison with experimental data shows that the first model, involving neutral Be interstitials in InGaAs and singly positively charged Be interstitials in InP, gives a better description than the second one, using neutral Be interstitials in InGaAs and InP.

1. Introduction

A highly doped base layer is known to be vital for high performance of InP/InGaAs double-heterojunction bipolar transistors (DHBTs), but the post-growth technological processes could cause an important redistribution of Be, commonly employed as the base dopant for InGaAs. This can significantly degrade device performance.

Little previous work on Be diffusion in InP epilayers or in InGaAs/InP heterostructures has been carried out [1, 2]. Nevertheless, a 'kick-out' model has proved successful in explaining experimental profiles [2]. In this letter we describe results on Be diffusion in the InGaAs/InP system during post-growth rapid thermal annealing (RTA).

2. Experimental procedure

All samples reported on here were grown by gas-source molecular beam epitaxy (GSMBE) on semi-insulating ⟨100⟩ InP substrates in a Vacuum Generators V80 system from VG Semicon. They each consist of a 0.2 μm Be-doped (3×10^{19} cm^{-3}) $In_{0.53}Ga_{0.47}As$ layer sandwiched between 0.5 μm InP undoped layers. The samples were grown at a rate of 0.8–2.0 μm h^{-1} with a V/III flux ratio of 5 and a substrate temperature around 500 °C.

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The post-growth RTA was performed in a halogen-lamp furnace, ADDAX 1000M, using flowing gas (Ar + 10% H_2).

The secondary-ion mass spectrometry (SIMS) measurements were made with a Cameca IMS-4F instrument using a 5.5 keV O_2^+ beam. The sputtered area was $250 \times 250\ \mu m^2$ and the area analysed had a diameter of 60 μm.

3. Results and discussion

In this work we found a strong segregation at the heterojunctions yielding a Be concentration in InGaAs about an order of magnitude higher than that in InP (figure 1). On the other hand, the absence of Be concentration spikes near the heterojunctions demonstrates that no Be gettering occurs in our case.

To obtain quantitative data fits, two kick-out models of the substitutional–interstitial diffusion (SID) mechanism were considered. The two models are based on the neutral Be interstitial species Be_i^0 and the singly positively charged In, Ga self-interstitials I_{III}^+ in $In_{0.53}Ga_{0.47}As$ [3]; however, in InP the first model involves the singly positively charged Be interstitial species Be_i^+ [1] with the doubly positively charged In self-interstitials I_{III}^{2+} and the second model uses, as in $In_{0.53}Ga_{0.47}As$, the neutral Be interstitial species Be_i^0 with the singly positively charged In self-interstitials I_{III}^+, according to the following diffusion reaction:

$$Be_i^{n+} \overset{K}{\Leftrightarrow} Be_s^- + I_{III}^{r+} \tag{1}$$

where $n = 0$, $r = 1$ in the ternary layer for the two models; $n = 1$, $r = 2$ and $n = 0$, $r = 1$ in the binary layers for the first and the second models, respectively. Be_s^- and K stand for the singly negatively ionized Be substitutionals and the reaction constant, respectively.

The diffusion differential equations for Be and group III mobile species, including the Fermi-level effect, the electric field produced by the charge distribution and the bulk self-interstitial generation/annihilation, for each model, were solved numerically, using the explicit finite-difference method [3].

According to the segregation, maximal total Be concentrations in the range 2.5×10^{18}–3.0×10^{18} cm^{-3} for temperatures in the range 700–900 °C, correspondingly, were used for the InP.

The conditions that the flux of diffusing species leaving the InGaAs layer is equal to that joining the InP layer, in view of the fact that there is no accumulation of diffusing substance at the boundaries, were applied as the boundary conditions at the InGaAs/InP interfaces in our simulations. In addition to that, ratios of the interface Be interstitial concentration in InP to that in InGaAs in the ranges 12.0–1.0 (model 1) and 15.0–2.30 (model 2) for temperatures in the range 700–900 °C correspondingly, and also ratios of the interface group III self-interstitial concentration in InP to that in InGaAs in the ranges 0.25–0.04 (model 1) and 0.20–0.05 (model 2) for temperatures in the range 700–900 °C correspondingly, were introduced in the boundary conditions as fitting parameters [4].

In order to consider the Be diffusion exclusively after growth, the SIMS depth profile for as-grown sample (see figure 1) was used as the initial concentration distribution curve in our simulations.

For InGaAs we used the same diffusion parameter values as have been found in the case of ternary homojunctions [3]. For InP layers, the diffusion parameters (Be interstitial equilibrium concentration C_i^{eq}, intrinsic self-interstitial equilibrium concentration $C_I^{eq}(n_i)$, Be interstitial diffusivity D_i, group III self-interstitial diffusivity D_I and group III self-interstitial annihilation/generation rate coefficient k_I) were optimized to give a best fit for experimental profiles.

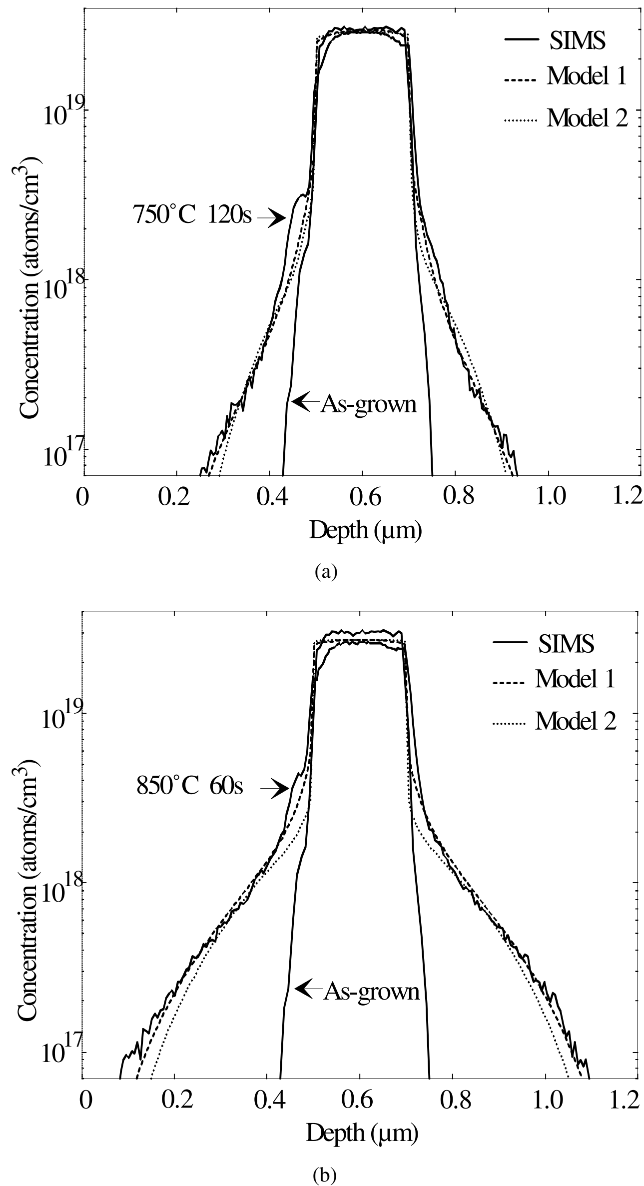

Figure 1. The Be SIMS data and simulated results for (a) $T = 750$ °C, 120 s; (b) $T = 850$ °C, 60 s.

The intrinsic carrier concentration $n_{\mathrm{i}} = 5.05 \times 10^{15} \times T^{3/2} \exp(-0.76\ \mathrm{eV}/k_B T)\ \mathrm{cm}^{-3}$ in InP has been calculated as in the case of InGaAs [3].

The parameters $C_{\mathrm{I}}^{\mathrm{eq}}(n_{\mathrm{i}})$, D_{i}, D_{I} and k_{I} for InP, listed in table 1 (model 1) and table 2 (model 2), satisfy to Arrhenius law (except the k_{I}-value for 700 °C). They are given in table 3.

Figures 1(a), 1(b) show the Be SIMS data obtained for the samples which were annealed at the temperatures of 750 and 850 °C for 120 and 60 s, respectively, as well as the simulated Be curves corresponding to the two models.

It can be seen that the first model gives better fits than the second model.

Table 1. The parameters used for the simulations of InP by the first model.

RTA T (°C)	C_i^{eq} (cm^{-3})	n_i (cm^{-3})	$C_I^{eq}(n_i)$ (cm^{-3})	D_i (cm^2 s^{-1})	D_I (cm^2 s^{-1})	k_I (s^{-1})
700	2.8×10^{17}	1.8×10^{16}	2.3×10^{11}	3.7×10^{-12}	3.2×10^{-12}	3.0
750	5.4×10^{17}	3.0×10^{16}	1.1×10^{12}	9.0×10^{-12}	7.9×10^{-12}	0.4
800	6.5×10^{17}	4.8×10^{16}	4.4×10^{12}	2.0×10^{-11}	1.8×10^{-11}	0.9
850	7.7×10^{17}	7.4×10^{16}	1.6×10^{13}	4.1×10^{-11}	3.8×10^{-11}	2.0
900	9.0×10^{17}	1.1×10^{17}	5.0×10^{13}	7.9×10^{-11}	7.5×10^{-11}	4.0

Table 2. The parameters used for the simulations of InP by the second model.

RTA T (°C)	C_i^{eq} (cm^{-3})	n_i (cm^{-3})	$C_I^{eq}(n_i)$ (cm^{-3})	D_i (cm^2 s^{-1})	D_I (cm^2 s^{-1})	k_I (s^{-1})
700	2.0×10^{17}	1.8×10^{16}	5.2×10^{12}	2.0×10^{-13}	6.0×10^{-14}	0.5
750	3.5×10^{17}	3.0×10^{16}	1.8×10^{13}	6.0×10^{-13}	2.0×10^{-13}	0.1
800	4.9×10^{17}	4.8×10^{16}	5.6×10^{13}	1.6×10^{-12}	6.0×10^{-13}	0.2
850	6.7×10^{17}	7.4×10^{16}	1.6×10^{14}	3.9×10^{-12}	1.6×10^{-12}	0.5
900	9.0×10^{17}	1.1×10^{17}	4.0×10^{14}	9.0×10^{-12}	4.0×10^{-12}	1.0

Table 3. The parameters $C_I^{eq}(n_i)$, D_i, D_I and k_I for InP.

InP (model 1)	InP (model 2)
$C_I^{eq}(n_i) = 1.18 \times 10^{25} \exp(-2.65\ \mathrm{eV}/k_B T)$ cm^{-3}	$C_I^{eq}(n_i) = 6.01 \times 10^{23} \exp(-2.14\ \mathrm{eV}/k_B T)$ cm^{-3}
$D_i = 2.32 \times 10^{-4} \exp(-1.51\ \mathrm{eV}/k_B T)$ cm^2 s^{-1}	$D_i = 9.96 \times 10^{-4} \exp(-1.87\ \mathrm{eV}/k_B T)$ cm^2 s^{-1}
$D_I = 3.47 \times 10^{-4} \exp(-1.55\ \mathrm{eV}/k_B T)$ cm^2 s^{-1}	$D_I = 3.00 \times 10^{-3} \exp(-2.07\ \mathrm{eV}/k_B T)$ cm^2 s^{-1}
$k_I = 2.65 \times 10^{7} \exp(-1.59\ \mathrm{eV}/k_B T)$ s^{-1}	$k_I = 6.62 \times 10^{6} \exp(-1.59\ \mathrm{eV}/k_B T)$ s^{-1}

4. Conclusions

We investigated the diffusion of Be InGaAs/InP heterostructures suitable for DHBT fabrication. The experimental profiles were simulated by adopting kick-out models, and taking into account the boundary conditions and the segregation phenomena at the interfaces.

The kick-out model using Be_i^0 in InGaAs and Be_i^+ in InP gives better fits than the kick-out model based on Be_i^0 in InGaAs and InP.

References

[1] Panish M B, Hamm R A, Ritter D, Luftman H S and Cotell C M 1991 *J. Cryst. Growth* **112** 343

[2] Chen C-H, Gösele U M and Tan T Y 1999 *Appl. Phys.* A **68** 9

[3] Ketata K, Ketata M, Koumetz S, Marcon J and Masmoudi M 1998 *Modell. Simul. Mater. Sci. Eng.* **6** 747

[4] Crank J 1999 *The Mathematics of Diffusion* (Oxford: Oxford University Press)