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1.2 K Shubnikov–de Haas measurements and self-consistent calculation of silicon spreading in δ - and slab-doped $In_{0.53}Ga_{0.47}As$ grown by molecular beam epitaxy

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Magnetotransport measurements are reported for $In_{0.53}Ga_{0.47}As$ layers grown by molecular beam epitaxy (MBE) at different substrate temperatures (T_s) and either δ - or slab-doped with Si. Multiple subband densities deduced from the Fourier analysis of 1.2 K Shubnikov–de Haas measurements are compared with those derived from self-consistent calculations which include nonparabolicity and the doping profile width w_{Si} as a fitting parameter. Significant spreading of the Si donors away from the doping plane is deduced for deposition at $T_s \approx 520$ °C, while no measurable migration is inferred for $T_s \leq 470$ °C, leading to near-ideal δ -doping behavior. Contrary to previous results [McElhinney *et al.*, J. Cryst. Growth **150**, 266 (1995)], no evidence for amphoteric behavior has been found for Si areal densities up to 4×10^{12} cm⁻². © 1996 American Institute of Physics. [S0003-6951(96)00707-0]

Atomic plane or δ -doping of III–V semiconductors with Si during molecular beam epitaxial (MBE) growth is used in the fabrication of nonalloyed Ohmic contacts,¹ in δ -doped Schottky-gate field effect transistors (FETs),² and lattice matched and pseudomorphic high electron mobility transistors (HEMTs)^{3,4} for fast electronic devices. Many studies of Si δ -doping in GaAs and AlGaAs have been reported^{5–7} but data for InGaAs^{8,9} and InAlAs is more limited despite the importance of these ternaries for ultrahigh frequency and ultra-low-noise devices based on InP.

In this letter, a study of the spreading of Si in δ - and thin slab-doped In_{0.53}Ga_{0.47}As grown lattice matched on InP by MBE at different substrate temperatures (T_s) is reported, extending earlier work⁸ which described the first application of Shubnikov-de Haas measurements and self-consistent calculations to this material system. The growth conditions for near-ideal δ -doping and for the controlled incorporation of Si donors distributed uniformly in thin slabs of predetermined thickness are established. The free-electron concentrations n_i in the occupied subbands (i=0,1,2,...) of the confinement potential associated with the positively charged Si donors are deduced from a Fourier analysis of Shubnikov-de Haas measurements. Since the relative occupancies of the lower energy subbands are sensitive to the width of the donor profile, w_{Si} ,^{10,11} the Si distribution can be estimated from a comparison of the experimental values of n_i and the subband ratio $n_{i=0}/n_{i=1}$ with those determined from a sequence of self-consistent calculations in which w_{Si} is used as a fitting parameter. The multi-subband character of δ - and slab-doped InGaAs is more pronounced than in GaAs due to its smaller effective electron mass and higher dielectric constant, and in consequence nonparabolicity¹² must be included to improve the accuracy of the analysis.

The InGaAs layers illustrated in Fig. 1 were grown at 1.0 μ m/h on Fe-InP(100) substrates in Varian MBE systems (designated machines "A" and "B"), both fitted with Varian arsenic crackers. The structures were designed to allow a distinction between dopant spreading caused by diffusion and by surface segregation. A constant As_2 flux of $\approx 1.9 \times 10^{15}$ molecules cm⁻² s⁻¹ was used, corresponding to \approx 6 times the minimum required to grow GaAs at a rate of 1 μ m/h and a temperature of 580 °C with a (2×4)(100) Asstable surface. The Ga and In fluxes were calibrated by RHEED intensity oscillations and the substrate temperature was estimated with an optical pyrometer. Three distinct InGaAs(100) surface reconstructions were observed along the [011] azimuth for the As₂ flux used; a (1×3) for $T_s \leq 470$ °C, a (2×3) for 470 °C $\leq T_s \leq 500$ °C and a (2×4) for $T_s \ge 500$ °C. These helped to set the growth conditions from run-to-run since the pyrometer reading was influenced by radiation from the group III furnaces. The InGaAs surface was exposed to the As₂ flux for the deposition of the Si δ layers and during the growth interrupts of 300 s required to lower and raise T_s . The Si furnace was calibrated with both low magnetic field Hall and high magnetic field Shubnikov-de Haas effect measurements of the free electron density in uniformly doped GaAs and In_{0.53}Ga_{0.47}As layers. The Si cell temperature was set to give an areal Si density of 3×10^{12} cm⁻² through 20 monolayers (ML) of InGaAs grown at 1 μ m/h. The same Si furnace temperature was then used for δ -doping with the growth interrupt time adjusted to give the required sheet Si density. 0.5 μ m thick undoped InGaAs buffer and cap layers grown at $T_s = 500-520$ °C

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FIG. 1. Schematic diagrams to show the structures and temperature profiles of MBE grown $In_{0.53}Ga_{0.47}As~\delta$ - and slab-doped with Si.

were common to all the structures except sample A951 which was grown entirely at 460 $^{\circ}$ C.

Shubnikov-de Haas measurements were performed at 1.2 K in the dark using a 13 T superconducting magnet on Hall bars with a 3:1 length to width ratio. The magnetoresistance data were numerically differentiated, expressed in reciprocal magnetic field and then frequency analyzed by fast Fourier transform (FFT) techniques. The peaks at frequency v_i in a FFT spectrum are related to the subband densities n_i , assuming unresolved spin splitting, by the expression $n_i=2ev_i/h$ where *e* is the electronic charge and *h* is Planck's constant. The total carrier concentration n_s is the sum of the individual electron concentrations n_i of all the observed subbands, $n_s = \sum_i n_i$.

The amplitude spectra for two δ -doped samples with areal Si densities of 2×10^{12} cm⁻² grown at 420 °C (B618) and 505 °C (B602) are shown in Fig. 2. The higher frequency of the i=0 peak for B618 represents a larger electron concentration n_0 in its lowest occupied subband compared with the value of n_0 for B602. The resultant reductions in n_i ($i \ge 1$) for B618 are reflected in a shift to lower frequencies of the $i \ge 1$ peaks and an increase in the subband ratio $n_{i=0}/n_{i=1}$ compared with the corresponding values for B602. The experimental values of n_i and $n_{i=0}/n_{i=1}$ for InGaAs samples both δ - and slab-doped with Si are shown in Table I, and compared with those calculated self-consistently assuming either a uniform (UD) or a Gaussian (GD) dopant distribution. Nonparabolicity has been included in the calculations within the limitations of the three-band Kane model.¹² The relative occupancies of the lower energy subbands are sensitive to the width of the doping profile as reported for GaAs δ -doped with Si.^{10,11} The total carrier concentrations predicted from theory include small contributions from the highest subbands ($\approx 1\%$) which are not detected by the Shubnikov-de Haas measurements. For the δ -layer grown at 505 °C (B602) the best-fit between theory and ex-



FIG. 2. Fast Fourier transform amplitude spectra for two δ -doped In_{0.53}Ga_{0.47}As samples with areal Si densities of 2×10^{12} cm⁻² where the δ -doped section is deposited at either 420 °C (B618) or 505 °C (B602).

periment is obtained for w_{Si} =45 ML (UD) and 40 ML (GD) (full width at 1/e maximum) indicating significant spreading of the Si donors away from the doping plane. The data show that a reduction in T_s from 505 to 420 °C (B618) appears to suppress the Si spreading to create a narrow doping profile. Note, that this is achieved by keeping the substrate temperature at 420 °C during the δ -layer deposition and the growth of 20 ML of undoped material only. The profile thus appears to be unaffected by the subsequent growth of the 0.5 μ m thick cap layer at 520 °C [Fig. 1(d)]. For the 4×10^{12} cm $^{-2}\delta$ -layer grown at 520 °C [B535, Fig. 1(a)], theory and experiment agree for w_{Si} =36 ML (UD) and 32 ML (GD), pointing once again to significant spreading of the Si donors away from the original doping plane. No migration of the Si donors is inferred from the data for the 4×10^{12} cm⁻² δ -layer grown at 470 °C [B610, Fig. 1(b)], showing that a decrease in T_s from 520 °C of only 50 °C is sufficient to eliminate spreading. As with sample B618, the near-ideal dopant confinement is achieved despite the growth of the 0.5 μ m undoped cap layer at 520 °C, providing indirect evidence that surface segregation is the principal mechanism contributing to the redistribution of Si for $T_s \ge 470$ °C. Self-consistent calculations predict a Fermi energy 190 meV above the Γ -conduction band minimum for an areal density of 4×10^{12} cm⁻² active Si donors confined to 2 ML. This is well below the L-conduction band minimum $(E_L - E_\Gamma = 550 \text{ meV})$, making the three-band model a reasonable approximation.

The absence of dopant spreading at low growth temperatures can be verified by comparing the experimental and theoretical values of n_i and $n_{i=0}/n_{i=1}$ for samples in which the Si dopant atoms are deliberately deposited within a thin slab of known thickness, and where w_{Si} for the selfconsistent calculations is then set to the physical thickness of the slab. Two samples [A951, Fig. 1(e) and A952, Fig. 1(f) with buffer and cap layers grown at 460 and 520 °C respectively], were doped with 3×10^{12} cm⁻² Si atoms distributed through 20 ML of InGaAs grown at 460 °C. The agreement between experiment and theory for both layers with $w_{Si}=20$ ML (see Table I) is excellent suggesting that at this overall doping density a deposition temperature of 460 °C is

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TABLE I. Growth conditions, Shubnikov-de Haas data and self-consistent calculations for δ - and slab-doped In_{0.53}Ga_{0.47}As grown by MBE. n_i (*i* = 0,1,2,3,...) are the electron densities in the subbands expression in units of $\times 10^{12}$ cm⁻²; $n_s = \sum_i n_i$; the subband ratio $n_{i=0}/n_{i=1}$ indicates the degree of confinement of the Si atoms. UD refers to the width w_{si} used in the self-consistent calculations when the Si atoms are assumed to have a uniform density distribution; GD refers to the full width at 1/e maximum for a Gaussian profile.

Sample No.	Deposition temperature (°C) Reconstruction	Subband densities, $\times 10^{12}$ cm ⁻²								Subband
			n_0	n_1	n_2	n_3	n_4	n_5	n_s	$n_{i=0}/n_{i=1}$
B602	505	Experiment	1.17	0.55	0.25	0.09			2.06	2.127
	(2×4)	45 ML (UD)	1.191	0.561	0.234	0.090	0.024		2.100	2.124
		40 ML (GD)	1.185	0.560	0.240	0.090	0.024		2.100	2.114
B618	420	Experiment	1.35	0.51	0.22	0.07			2.15	2.647
	(1×3)	2 ML (UD)	1.365	0.509	0.229	0.077	0.021		2.200	2.681
		2 ML (GD)	1.362	0.514	0.224	0.078	0.021		2.200	2.651
B535	520	Experiment	2.17	1.10	0.53	0.25	0.09		4.14	1.973
	(2×4)	36 ML (UD)	2.202	1.120	0.513	0.228	0.083	0.023	4.170	1.966
		32 ML (GD)	2.189	1.114	0.526	0.231	0.086	0.023	4.170	1.965
B610	470	Experiment	2.49	1.02	0.49	0.20	0.07		4.27	2.441
	(1×3)	2 ML (UD)	2.500	1.018	0.491	0.199	0.075	0.017	4.300	2.459
		2 ML (GD)	2.496	1.021	0.490	0.200	0.075	0.018	4.300	2.444
A951	460	Experiment	1.71	0.72	0.31	0.12			2.86	2.375
	(1×3)	20 ML (UD)	1.701	0.713	0.319	0.123	0.038	0.005	2.900	2.385
		25 ML (UD)	1.675	0.730	0.323	0.127	0.040	0.006	2.900	2.295
A952	460	Experiment	1.77	0.75	0.33	0.11		•••	2.96	2.360
	(1×3)	20 ML (UD)	1.755	0.738	0.333	0.130	0.041	0.006	3.000	2.386

low enough to confine the Si to the intended region. For comparison, theoretical data for Si donors assumed to be uniformly distributed through 25 ML is also presented in Table I. The discrepancy between theory and experiment in this case is significant and an upper limit of <5 ML on the total spreading can therefore be set with confidence. These results demonstrate the precision with which spreading of Si dopant atoms in InGaAs can be estimated through a combination of Shubnikov–de Haas measurements and self-consistent calculations.

In summary, Si spreading in both δ - and slab-doped In_{0.53}Ga_{0.47}As grown by MBE at different substrate temperatures has been reported. Significant spreading (≥ 100 Å) away from the original doping plane is concluded for Si densities up to 4×10^{12} cm⁻² when the δ -doped structure is deposited at 520 °C. No spreading away from the δ-doped plane or outside a thin slab of predetermined thickness is resolved for $T_s \leq 470$ °C, even when a 0.5 μ m thick cap layer is subsequently grown at \approx 520 °C. This leads to the conclusion that Si spreading results predominantly from surface segregation and that diffusion during growth up to \approx 520 °C is negligible. There is no measurable compensation at areal Si densities up to 4×10^{12} cm⁻², modifying one conclusion drawn in Ref. 8 where the intended Si dopant density was overestimated by a factor of ≈ 1.5 . Finally, the applicability of the self-consistent calculations would be enhanced by taking into account the asymmetry of the Si profile caused by the surface segregation.

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