The effect of oxygen incorporation in semi-insulating $(Al_xGa_{1-x})_yIn_{1-y}P$

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Oxygen-doped, semi-insulating layers of $(Al_xGa_{1-x})_yIn_{1-y}P$ with x = 0.4 were grown on GaAs using organometallic vapor phase epitaxy (OMVPE). Secondary-ion mass spectrometry measurements show that the oxygen incorporation is proportional to the flow rate of O₂ into the OMVPE reactor. Two-terminal metal-insulator-semiconductor devices were fabricated and used to evaluate the electrical characteristics of the $(Al_xGa_{1-x})_yIn_{1-y}P$ bulk behave like *DX* centers, and are believed to be related to residual Si contamination. Increasing the oxygen concentration in the $(Al_xGa_{1-x})_yIn_{1-y}P$ layer decreases the trap concentration by the formation of oxygen complexes with the Si atoms.

Oxygen has long been associated with semi-insulating behavior in III-V compound semiconductors, but the role of oxygen is still not clearly understood. In GaAs, oxygen has been linked to an electrically active Ga-O-Ga defect and to inactive interstitial atoms.¹ Semi-insulating $Al_xGa_{1-x}As$ has been produced by the incorporation of oxygen in layers grown by molecular beam epitaxy $(MBE).^2$ The characteristics of high-resistivity $(Al_xGa_{1-x})_{\nu}In_{1-\nu}P$ were previously reported for organometallic vapor phase epitaxy (OMVPE) layers with no intentional oxygen incorporation.³ In this letter, the behavior of semi-insulating $(Al_xGa_{1-x})_yIn_{1-y}P$ grown by OMVPE with controlled oxygen incorporation is reported.

The epitaxial layers were grown on $(100) n^+$ -GaAs substrates. A GaAs buffer layer with a nominal thickness of 2 μ m was grown with no intentional doping, followed by the $(Al_xGa_{1-x})_yIn_{1-y}P$ layer with a nominal thickness of 0.5 μ m. The composition of the $(Al_xGa_{1-x})_yIn_{1-y}P$ was determined for each sample using energy-dispersive spectroscopy. For the three samples discussed here, the subscript x was in the range 0.36–0.42, while the subscript y was about 0.58. The resulting lattice mismatch to GaAs is less than 0.5%. Incorporation of oxygen was controlled by varying the flow rate of O₂ into the reactor in the range 0–100 sccm.

The oxygen concentration in the $(Al_xGa_{1-x})_yIn_{1-y}P$ layers was measured with a Perkin– Elmer PHI-6300 secondary-ion mass spectrometry (SIMS) system using a Cs⁺ ion beam. A 10^{15} cm⁻² dose of O₂ was implanted into each sample at an energy of 15 keV. SIMS depth profiles were then acquired through the implanted region to the bulk material, and the signal in the implanted region used to quantify the level of oxygen in the bulk. The minimum detected oxygen concentration was 3.7×10^{17} cm⁻³, which is comparable to the detection limit for oxygen in Al_xGa_{1-x}As.⁴

Figure 1 shows the measured concentration of oxygen in the $(Al_xGa_{1-x})_yIn_{1-y}P$ layers for three samples, plotted as a function of the O₂ flow rate during growth. The error estimate of the SIMS measurement is mainly due to uncertainty in the depth of the sputtered craters. A line with slope $\frac{1}{2}$ is shown to connect the data points within the error estimate. If the oxygen is incorporated as isolated interstitial atoms, the reaction from the diatomic molecule would be

$$O_2 = 2O_b$$
 (1)

with the equilibrium constant for this reaction given by

$$K = \frac{[O_i]^2}{p_{O_2}}.$$
 (2)

Here p_{O_2} is the partial pressure of O_2 in the OMVPE reactor and the square bracket notation is used to indicate the concentration of a species. The interstitial oxygen (O_i) will be in equilibrium with substitutional oxygen occupying a group-V lattice site (O_P) , with the total oxygen concentration given by

$$[O] = [O_i] + [O_p].$$
(3)

Because O_2 is present in very dilute quantities, the partial pressure is proportional to the flow rate of O_2 into the reactor. Combining this with Eqs. (2) and (3) gives

$$[O] \propto f_{O_2}^{1/2}, \tag{4}$$

where f_{O_2} is the O₂ flow rate. The square-root dependence of the total oxygen concentration on the O₂ flow rate is consistent with the slope of the line shown in Fig. 1.

To evaluate the effect of oxygen on the electrical properties of $(Al_xGa_{1-x})_yIn_{1-y}P$, two-terminal metal-insulator-semiconductor capacitors were fabricated. The Au-Cr gates were prepared by evaporation through a metal mask with circular contacts of 62.5-, 125-, 250-, and 500- μ m diameter. Ohmic contact to the n^+ substrate was formed by spark alloying a Sn-doped Au wire. The capacitancevoltage (*C-V*) characteristics of the devices were measured using a Hewlett–Packard HP-4284A Precision LCR meter under computer control.

In Fig. 2, the 1 MHz C-V curves for the three samples are shown as solid lines, normalized to the accumulation

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FIG. 1. Concentration of oxygen in the bulk of the $(Al_xGa_{1-x})_yIn_{1-y}P$ layer as measured by SIMS. The dotted line has slope $\frac{1}{2}$.

capacitance. For this measurement the bias was swept from +5 V to -20 V at a rate of 100 mV/s. Superimposed on the measured curves are fitted characteristics, shown as dotted curves. Because the intrinsic carrier concentration of GaAs is small, the generation of minority carriers is slow and inversion of the GaAs surface is unlikely. Therefore, the fitted curves are deep-depletion characteristics



FIG. 2. 1-MHz C-V plot for samples A, B, and C. The dotted curves are fitted deep-depletion characteristics.

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FIG. 3. Concentration of traps distributed uniformly in the bulk of the $(Al_xGa_{1-x})_yIn_{1-y}P$ layer. The trap concentration is calculated from the flatband voltage shift of the *C-V* curves shown in Fig. 2. The dotted line has slope (-1).

calculated by neglecting minority carriers.⁵ Each curve was fit by matching the measured accumulation capacitance, assuming a buffer layer doping of about 3.4×10^{15} cm⁻³ and adding a voltage shift.

The negative voltage shift of the C-V curves is due to positive charge trapped in the bulk of the $(Al_xGa_{1-x})_yIn_{1-y}P$ layer. For a uniform distribution of charge, the voltage shift is given by⁶

$$\Delta V = -\frac{qN_I d}{2C_I'}, \qquad (5)$$

where q is the electron charge, N_I the trap concentration in the $(Al_xGa_{1-x})_yIn_{1-y}P$ layer of thickness d, and C'_I the accumulation capacitance per unit area. A convenient reference point for determining ΔV is the flatband voltage V_{FB} , defined as the point where the measured capacitance satisfies the flatband condition.⁷ The voltage shift also includes the work function difference ϕ_{ms} between the metal and semiconductor, so that

$$\Delta V = V_{\rm FB} - \phi_{\rm ms}.\tag{6}$$

For a Cr gate and the *n*-type buffer layer doping, $\phi_{\rm ms} = 0.3$ V.

Figure 3 shows the trap concentration N_I in the $(Al_xGa_{1-x})_yIn_{1-y}P$ layer for the three samples, plotted as a function of the oxygen concentration measured in each sample. Of interest here is that the trap concentration decreases as the oxygen concentration increases, indicating that oxygen is not primarily responsible for the trap. Rather, a second species forms the trap, and then is reduced in concentration by the incorporation of oxygen. Si

is present as a contaminant in $(Al_xGa_{1-x})_yIn_{1-y}P$ layers grown by OMVPE in concentrations of about $10^{16}-10^{17}$ cm⁻³, which corresponds to the observed trap concentration. Furthermore, Si has been identified as a *DX* center in $(Al_xGa_{1-x})_yIn_{1-y}P$.⁸ It seems likely, therefore, that Si is responsible for the donor-like deep traps in the $(Al_xGa_{1-x})_yIn_{1-y}P$ layers.

To explain the reduction of the trap concentration in the presence of greater amounts of oxygen, the formation of a complex between Si and O is postulated. Such a complex has been observed in GaAs,⁹ where a Si donor on a Ga lattice site combines with interstitial oxygen, as expressed by

$$\mathrm{Si}_{\mathrm{Ga}}^{+} + \mathrm{O}_{\mathrm{F}} = \mathrm{SiO}^{-} + 2e^{+}. \tag{7}$$

Here e^+ represents a hole, necessary for charge neutrality. The equilibrium constant for this reaction is given by

$$K = \frac{p^2 [\text{SiO}^-]}{[\text{Si}^+][\text{O}_i]},$$
(8)

where p is the hole concentration. Since the Si concentration is fixed within the sample, the formation of a Si-O complex reduces the Si available to act as a Si-donor DXcenter. Using Eq. (8), this means that

$$[\operatorname{Si}^+] \propto [\operatorname{O}_i]^{-1}. \tag{9}$$

This inverse relationship gives a line with slope (-1) on a logarithmic plot. Such a line is shown in Fig. 3, showing that the formation of Si-O complexes is consistent with the observed data. Since the reaction is with the interstitial oxygen, which is electrically inactive, the complex formation does not affect the semi-insulating nature of the material.

In conclusion, semi-insulating $(Al_xGa_{1-x})_yIn_{1-y}P$ was grown by OMVPE with controlled amounts of oxygen added. Oxygen is incorporated into the $(Al_xGa_{1-x})In_{1-y}P$ in proportion to the amount of O₂ introduced into the reactor. C-V measurements showed a pronounced negative flatband voltage shift which decreased with increasing oxygen. A consistent explanation has been proposed in which charge is trapped in the $(Al_xGa_{1-x})_{\nu}In_{1-\nu}P$ bulk by Si-donor DX centers. Increasing the oxygen concentration in the $(Al_xGa_{1-x})In_{1-y}P$ layer decreases the DX center concentration by the formation of Si-O complexes.

The composition of the $(Al_xGa_{1-x})_yIn_{1-y}P$ layers were measured at the Analytical Lab of MCNC, Research Triangle Park, NC with the assistance of Richard Chapman. The SIMS analysis was performed at the Analytical Lab of MCNC by J. J. Lee and Mark Ray. This work was supported by the National Science Foundation under grant ECS-8701650.

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