A hybrid epitaxy method for InAs on GaP

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The interface formation mechanism during the molecular-beam epitaxy (MBE) of InAs/GaP has been studied with the aid of the In–Ga–P phase diagram. It is discovered that an initial dissolution and crystallization process similar to liquid phase epitaxy (LPE) may happen at sufficiently high temperature, resulting in a graded composition at the interface. Consequently, "parasitic LPE/MBE" is the name for this hybrid form of MBE. High-resolution TEM images confirm the existence of the interfacial layer in the sample grown at high temperature. The graded interface smears out the band offset and leads to a nonrectifying heterojunction. Low-temperature (LT) MBE growth can turn off the LPE component, enabling the growth of an abrupt interface. Based on this "LPE/MBE" model, a LT MBE technique is developed to grow an abrupt InAs/InGaP interface for heterojunction power Schottky rectifiers. The LT InAs/InGaP heterojunction demonstrates nearly ideal Schottky rectifier characteristics, while the sample grown at high temperature shows resistive ohmic characteristics. The LT InAs/InGaP Schottky diode also demonstrates good stability with respect to anneal temperature, similar to the InAs/GaP heterojunctions. [DOI: 10.1063/1.1808241]

Conventional high-power Schottky rectifiers are made from metal–semiconductor (MS) diodes.[1] A critical concern for high-power rectifiers is the thermal stability, because most power devices are inevitably subjected to high-temperature processing or joule heating during operation. The MS interface degrades severely at high temperature due to the intermixing and metal migration at the interface. As an alternative, an isotype *n-n* heterojunction can also work as a rectifier if a barrier is developed in the conduction band.[2] It is similar to the MS Schottky rectifier as a majority carrier device. For example, the InAs/GaP heterojunction grown by molecular-beam epitaxy (MBE) has demonstrated nearly ideal Schottky rectifier characteristics, in spite of the large lattice mismatch (~11%) between InAs and GaP.[3–7] Heavily doped *n*-type InAs is highly conductive and acts as a "metal" layer in this heterojunction Schottky rectifier. The InAs/GaP diodes also demonstrates better stability than the metal/GaP diodes after high temperature anneals, owing to the suppression of the interdiffusion across interfaces in large lattice-mismatched semiconductor systems. Therefore the InAs/GaP heterojunction provides a structure for the high-temperature power Schottky rectifier.

However, the performance of GaP-based power devices is limited by its low mobility. Direct band gap InGaP has better figure of merit for power devices than GaP.[8,9] The Baliga figure of merit (BFOM) has been widely used to evaluate semiconductor materials for high-power applications. Due to its wide band gap, high mobility ($\sim 3000\ \mathrm{cm^2/V\ s}$) and high breakdown electric field ($\sim 0.8\ \mathrm{MV/cm}$), InGaP has BFOM of 39 normalized to that of Si as 1. It means that a high-power rectifier made from InGaP will have a theoretical mobility limited on-resistance 39 times less than that of a Si rectifier with the same blocking voltage. Therefore, we studied the growth of InAs on InGaP lattice-matched to GaAs. Normal MBE of InAs on InGaP resulted in heterojunctions that were leaky. To address the issue of why the direct growth of InAs on InGaP resulted in leaky diodes, we studied the interface formation mechanism during MBE growth of InAs on GaP. The same analysis also applies to the MBE of InAs on InGaP.

For epilayer perfection reasons, an In-rich condition is used to initiate nucleation of InAs on GaP (and InGaP). During the initial In-rich phase of MBE, excess In forms a "liquid" layer on the surface of GaP, creating a liquid composition that is undersaturated with respect to liquid–solid phase equilibrium in the In–Ga–P phase diagram.[10–13] This undersaturation is relieved at high growth temperatures by the dissolution of GaP into the liquid In to form a ternary In–Ga–P liquid solution, until pseudoequilibrium is reached with the GaP substrate. Figure 1 shows the equilibrium between an In–Ga–P liquid (the square) and a ternary solid (the circle) on GaP substrate in a schematic In–Ga–P phase diagram. A tie line connects the compositions of the two phases that coexist at equilibrium. When the As flux is added to this liquid for the growth of InAs, it creates a supersaturation that is relieved by the crystallization of the liquid solution. As a result, an $In_xGa_{1-x}P_yAs_{1-y}$ layer grows at the GaP interface with a composition graded from being (Ga,P) rich at the GaP interface to being (In,As) rich at the last-to-freeze surface until finally the pure InAs composition is reached. After that, the InAs epilayer grows on the surface by "normal" MBE. Therefore, instead of forming an abrupt interface, a compositionally graded layer forms at the InAs/GaP interface during a high-temperature MBE growth. Since the initial GaP dissolution into the In surface layer and crystallization of this In–Ga–P "liquid" layer is similar to the liquid phase epitaxy (LPE) process, it is named "parasitic LPE/MBE" as a hybrid form of MBE. This graded layer growth

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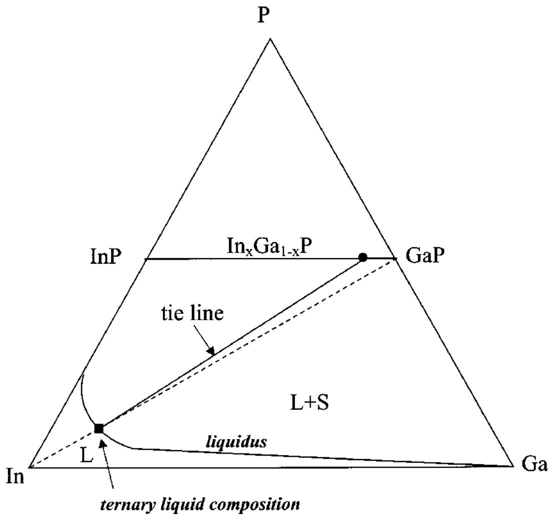

FIG. 1. An isothermal section of a schematic In–Ga–P phase diagram showing the equilibrium liquid and solid compositions.

mechanism is similar to the isothermal solution mixing growth in the LPE of $Ga_{1-x}Al_xAs$.[14,15]

The presence of the interfacial layer has been confirmed by the high-resolution TEM of the InAs/GaP interfaces grown at different temperatures, as shown in Fig. 2. Figure 2(a) is a sample grown at lower temperature (~300 °C) which shows clear abrupt interface with misfit dislocations

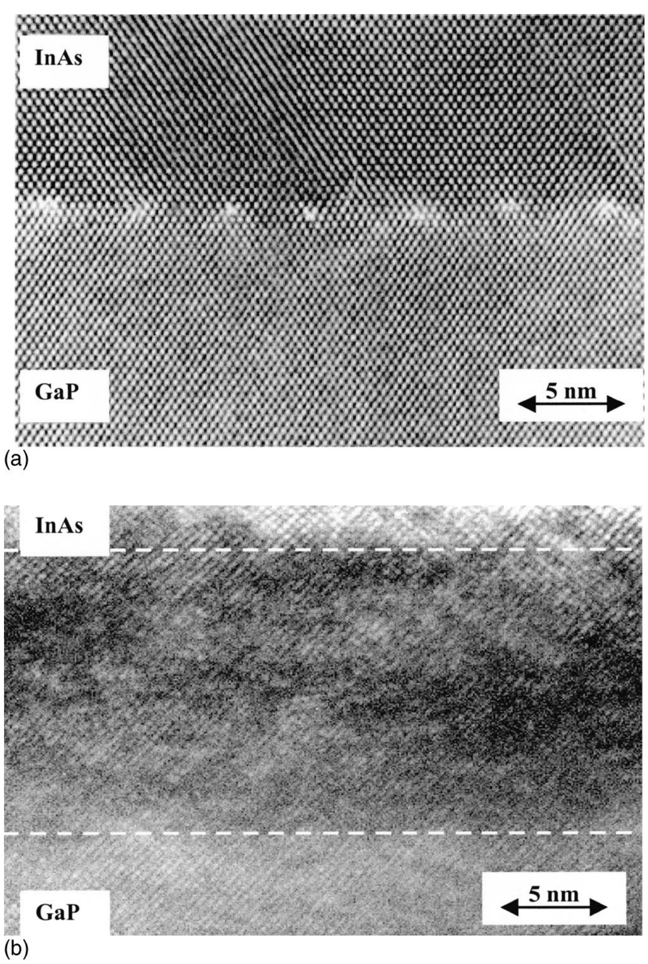

FIG. 2. High-resolution, cross-sectional TEM photomicrograph of InAs/GaP heterojunction grown at the temperature of 300 °C (a) and 500 °C (b).

indicated by the white dots at the interface. Figure 2(b) shows a sample grown at higher temperature (~500 °C) which has a "smeared" interfacial layer with a width of ~15 nm between InAs and GaP. The same LPE/MBE process can happen during the growth of InAs on InGaP at high temperature. As we can see from the In–Ga–P phase diagram in Fig. 1, the solubility of InGaP in liquid In is higher than that of GaP. Therefore, the initial LPE process is expected to produce a thicker interface graded layer for the InAs/InGaP structure than that for the InAs/GaP structure. The existence of a graded composition region in a heterojunction interface will smear out the band offset and lead to an electrically leaky diode. This explanation is consistent with the experimental observation of the leaky characteristics in InAs/InGaP heterojunctions grown at high temperature.

At low substrate temperatures, the liquidus line approaches pure In composition (the " In" corner in the phase diagram in Fig. 1), indicating lower solubility of GaP or InGaP in liquid In. When the temperature is sufficiently low, a thin liquid layer of almost pure In composition can exist in equilibrium with the GaP or InGaP substrate. So low-temperature growth can turn off the LPE components and allow normal MBE to form an abrupt interface that is needed for an ideal Schottky rectifier. Thus, a low-temperature MBE technique can be employed to grow abrupt InAs/GaP or InAs/InGaP heterojunctions. Since InGaP is superior to GaP for power device applications, we further applied this low-temperature MBE technique in the study of InAs/InGaP heterojunction Schottky rectifiers.

This LPE/MBE model is also tested by the electrical characteristics of the InAs/InGaP heterojunctions grown at both high and low temperatures. The samples were grown by a solid source MBE. A 2.0-μm-thick 3×10^{-16} cm^{-3} silicon (Si) doped InGaP layer was grown lattice-matched on a GaAs substrate with a 1.0 μm heavily doped GaAs buffer layer between these two layers. A 500-Å-thick 1×10^{19} cm^{-3} Si-doped InAs layer was grown on top of the InGaP layer at 250 °C (for samples grown at "low" temperature) and at 500 °C (for samples grown at "high" temperature). A thin $In_{0.75}Al_{0.25}As$ capping layer (50 Å) was grown on top of the InAs layer to minimize the decomposition of InAs during high-temperature anneals. TiAu contact was deposited using e-beam evaporator and patterned using lift-off for electrical characterization. Schottky rectifiers were fabricated by etching InAs in $1H_2O_2:3H_3PO_4:50H_2O$ using the patterned TiAu as an etching mask. A back-side ohmic contact was made of AuGeNi alloyed at 400 °C for 30 s in a rapid thermal annealer (RTA). No edge termination techniques were used. The effect of growth temperature on the electrical properties is compared on the two samples grown at 250 and 500 °C.

Current–voltage ($I-V$) characteristics were measured using an HP4156A parameter analyzer. Figure 3 shows the forward bias $I-V$ characteristics of the low-temperature (LT) InAs/InGaP heterojunction, high-temperature (HT) InAs/InGaP heterojunction, and TiAu/InGaP metal–semiconductor Schottky junction. The LT InAs/InGaP heterojunction shows linear $I-V$ characteristics over six orders of current magnitudes on the semi-logarithm scale, as shown by the solid line. The bend over at larger voltage is due to the series resistance. An ideality factor of 1.06 and a barrier height of 0.8 eV were calculated, by fitting the $I-V$ characteristics into the thermionic emission theory. On the reverse

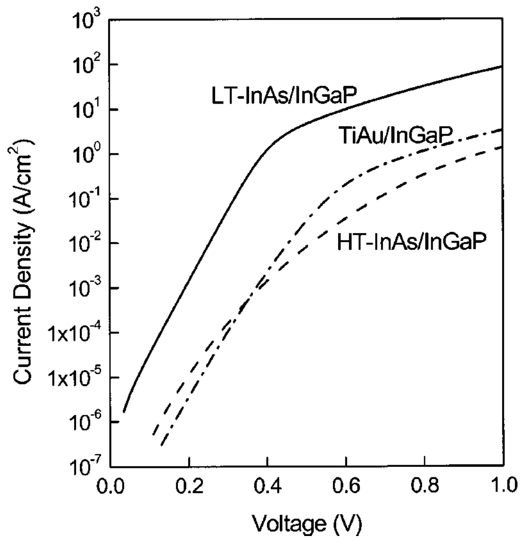

FIG. 3. Forward bias current–voltage characteristics of InAs/InGaP heterojunction rectifiers grown at low temperature (LT) and high temperature (HT).

bias side, the diode shows a soft breakdown and the maximum parallel plane electric field achieved is about 0.5 MV/cm. The TiAu/InGaP rectifier has shown similar Schottky diode characteristics. However, the InAs/InGaP sample grown at higher temperature (500 °C) shows resistive, ohmic characteristics, as shown by the dashed line in Fig. 3. The lower current in the HT sample is probably caused by higher series resistance in this device. These nonrectifying characteristics of the HT sample are expected from the LPE/MBE model.

The reliability of the LT InAs/InGaP heterojunction rectifiers has been studied by annealing the samples by RTA before metalization. The annealing was done in N_2 ambient for 1 min at temperatures between 500 and 700 °C. Samples were placed upside down on a supporting Si wafer in the RTA chamber and no cap layer was used. Figure 4 shows the forward bias $I-V$ characteristics of the samples before and after annealing at 50O, 600, and 700 °C, respectively. The LT InAs/InGaP heterojunction has maintained Schottky rectifying characteristics up to 700 °C with the same ideality factor. The difference on the current level is probably due to the slight change of the band offset after annealing. After 700 °C annealing, although some decomposition of InAs layer on the sample edge was observed, many devices still survived. This excellent reliability is thought to be due to the large lattice mismatch at the interface that effectively prevents the intermixing and interdiffusion at the interface, similar to the mechanism in the InAs/GaP heterojunction rectifiers.[16]

In summary, we investigated the origin of "leaky" InAs/InGaP heterojunction Schottky diodes formed via high temperature (500 °C) MBE. We present evidence that during the initial In-rich nucleation of InAs on either GaP or InGaP substrates, a thin liquid or liquid-like In-rich layer of In–Ga–P is formed which, upon supersaturation with the

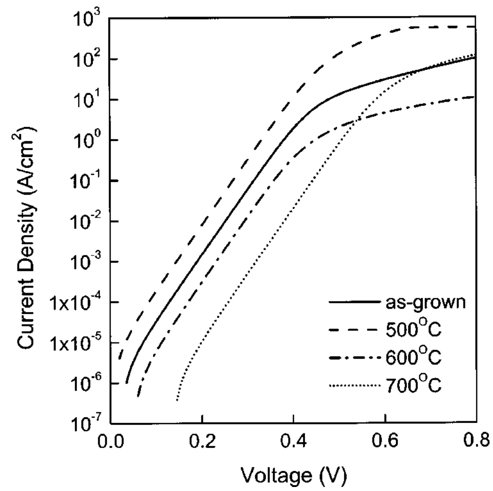

FIG. 4. Forward bias current–voltage characteristics of LT InAs/InGaP heterojunction rectifiers before and after annealing at 500, 600, and 700 °C, respectively.

MBE As source, causes the growth of a compositionally graded layer between the GaP substrate and the InAs epilayer formed by normal MBE. Since this graded layer forms by a process similar to alloy layers formed by LPE, we have named and modeled this process as "parasitic LPE/MBE." Using ternary phase diagram arguments, the "LPE/MBE" model explains the effect of growth temperatures on the electrical properties of the heterojunction Schottky rectifiers. To test the predictive ability of our model, we designed and tested a low-temperature (250 °C) MBE growth technique to form abrupt InAs/InGaP heterojunctions. The resulting LT InAs/InGaP heterojunctions show nearly ideal Schottky rectifier characteristics with an ideality factor of 1.06 and a barrier height of 0.8 eV. The reverse breakdown electric field of 0.5 MV/cm has been achieved without employing any edge-termination technique. The LT InAs/InGaP has shown excellent reliability and maintained the Schottky rectifier characteristics up to 700 °C.

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