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High-quality InAs$_y$P$_{1-y}$ step-graded buffer by molecular-beam epitaxy

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Relaxed, high-quality, compositionally step-graded InAs$_y$P$_{1-y}$ layers with an As composition of $y = 0.4$, corresponding to a lattice mismatch of $\sim 1.3\%$ were grown on InP substrates using solid-source molecular-beam epitaxy. Each layer was found to be nearly fully relaxed observed by triple axis x-ray diffraction, and plan-view transmission electron microscopy revealed an average threading dislocations of $4 \times 10^5 \text{ cm}^{-2}$ within the InAs$_{0.4}$P$_{0.6}$ cap layer. Extremely ordered crosshatch morphology was observed with very low surface roughness (3.16 nm) compared to cation-based In$_{0.7}$Al$_{0.3}$As/In$_x$Al$_{1-x}$As/InP graded buffers (10.53 nm) with similar mismatch and span of lattice constants on InP. The results show that InAs$_{1-y}$P$_{y}$ graded buffers on InP are promising candidates as virtual substrates for infrared and high-speed metamorphic III–V devices.

InAs$_{1-y}$P$_{y}$ alloys are of interest for both infrared optoelectronic and high-speed electronic device applications due to their wide range of band-gap energies from 0.36 eV to 1.35 eV and the large band offset energies possibly using InAs$_x$P$_{1-x}$/In$_x$Ga$_{1-x}$As heterostructures grown on InP. InAs$_{1-y}$P$_{y}$ alloys are also of interest for compositionally graded buffer applications, where the span of lattice constants between InP and InAs provides the opportunity for generating “virtual substrates” on InP to support a wide variety of lattice-mismatched devices based on In$_x$Ga$_{1-x}$As, In$_y$Al$_{1-y}$As, and InAs$_{1-y}$P$_y$. This is currently being explored for thermophotovoltaic (TPV) devices based on In$_x$Ga$_{1-x}$As, where the band gaps required for optimal TPV system conversion efficiencies in the range of 0.5–0.6 eV necessitate In$_x$Ga$_{1-x}$As compositions ($x = 0.69–0.81$) that generate a significant lattice mismatch with respect to the InP substrate. The use of an anion (group-V)-based alloy, such as InAs$_{1-y}$P$_y$ for compositionally graded buffers, compared with more common graded buffer alloy choices, such as In$_x$Ga$_{1-x}$As and In$_y$Al$_{1-y}$As, which can also bridge the lattice constant mismatch between active device layers and the InP substrate, offers a potential advantage since control of the growth rate (indium flux) is decoupled from control of the layer composition (As:P flux ratio). The addition of the group-V sublattice, as an independently controlled variable, has the effect of widening the parameter space for the growth of such graded buffers that is otherwise constrained for cation (group-III)-based graded buffers where growth rates and compositions are both dictated by the group-III sources. This is particularly advantageous for solid-source molecular-beam epitaxy (MBE) growth since optimizing the group-III fluence with respect to both composition and growth rate is extremely time consuming and would require substantial growth interruptions that may compromise interface quality. In this letter, we report the growth of high-quality relaxed InAs$_{1-y}$P$_y$ step-graded buffers by solid-source MBE that show great promise for virtual substrates applications.

InAs$_{1-y}$P$_y$ compositionally step-graded (four steps) layers with As mole fractions ($y$) from 0.05 to 0.40 were grown on (100) semi-insulating InP substrates using solid-source MBE equipped with valved cracker sources for arsenic and phosphorus. Substrate oxide desorption was done at 510 °C under a phosphorus overpressure of $\sim 1 \times 10^{-5}$ Torr, which was confirmed by the observation of a strong (2 $\times$ 4) reflection high-energy electron diffraction (RHEED) pattern, indicative of a clean (100) InP surface. An initial 0.2 $\mu$m thick undoped InP buffer layer was then deposited to generate a smooth surface at $\sim$485 °C under a stabilized P$_4$ flux prior to the growth of InAs$_x$P$_{1-x}$ step-graded buffers. After InP growth, the P$_4$ flux was reduced to the required value for the InAs$_{1-y}$P$_y$ growth and the As valve was opened before introducing In into the growth chamber. The exposure time of As on the InP substrate was minimized in order to avoid the formation of an InAsP interlayer due to As–P exchange on the InP surface. For all InAs$_{1-y}$P$_y$ layers, the growth rate was 0.75 monolayers/s, as determined by RHEED intensity oscillations at a constant substrate temperature of 485 °C controlled by a pyrometer-based feedback control system. The first three undoped step-graded layers were each grown to a thickness of 0.4 $\mu$m, followed by a 1.7 $\mu$m thick n-type (Si-doped) InAs$_{0.4}$P$_{0.6}$ layer with $n \sim 3 \times 10^{16}$ cm$^{-3}$ for char-

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acterization purposes. The total mismatch between the cap layer and the InP substrate is $1.3\%$.

Figure 1 shows a cross-sectional transmission electron microscopy (XTEM) image of a typical InAs$_{0.4}$P$_{0.6}$/InAs$_{y}$P$_{1-y}$/InP step-graded buffer structure. The compositions shown in Fig. 1 were determined using triple axis x-ray diffraction (described below). The image of Fig. 1 shows a high contrast at the graded buffer layer interfaces due to misfit dislocations with no threading dislocations (TDs) observable in the 1.7 $\mu$m thick InAs$_{0.4}$P$_{0.6}$ cap layer using XTEM. Hence, to accurately quantify the dislocation density, plan-view transmission electron microscopy (TEM) measurements were performed, the results of which are shown in Fig. 2. By considering several fields of view, the average TD density (TDD) in the relaxed InAs$_{0.4}$P$_{0.6}$ cap was found to be $4 \times 10^6$ cm$^{-2}$. It should be noted that both etch pit density (EPD) measurements using AgNO$_3$:CrO$_3$:HF:H$_2$O (A–B etch) and electron-beam-induced current measurements on InGaAs $p$–$n$ junctions grown on the InAsP buffer were also performed. These measurements revealed matching values of $\sim 1 \times 10^5$ cm$^{-2}$ for EPD and dark spot density, respectively, in substantial disagreement with the plan-view TEM results and significantly underestimating the true TDD value. This exemplifies the general difficulty in quantifying TDD values in high-quality relaxed buffers.

The relaxation state of the InAs$_{y}$P$_{1-y}$ graded buffer structure was evaluated using high-resolution triple axis x-ray diffraction measurements. Figure 3 shows reciprocal space maps (RSMs) for the (004) and (224) reflections. From the RSM in Fig. 3(a), the diffraction intensity maximum for each layer in the buffer is almost centered on the substrate reciprocal lattice point (along the vertical line drawn here), indicating minimum lattice tilt with respect to the substrate. For the asymmetric (224) reflection in Fig. 3(b), the intensity contours corresponding to the step-graded buffer and the final 1.7 $\mu$m layer makes an angle of $\sim 32^\circ$ with respect to the substrate reciprocal lattice intensity contours indicating that the material is almost fully relaxed, since the angle between (004) and (224) is $\sim 35^\circ$. To further quantify the relaxation of each layer, the lattice parameters in the growth plane $a_\|$, and in the growth direction $a_\perp$ were determined. The relaxed lattice constant, $a_\|$ and the relaxation, $R$ of the layers were evaluated using $Q_x = 2\lambda/\left(2a_\|\right)$, $Q_y = 2\lambda/\left(2a_\perp\right)$, and $Q_z$, expressed in terms of reciprocal lattice units. Here, $\lambda$ is the x-ray wavelength.
and InAs 0.4 P 0.6 layers in the buffer stack, respectively, noting percent relaxation was determined to be InAs 0.4 P 0.6 surface. The expected crosshatch morphology that typical atomic force microscopy ~ AFM ~ reveals a rms roughness that is more than three times lower, 3.16 nm, for the InAsP graded buffer as opposed to more than 10.53 nm for the graded InAlAs structure. The peak-to-peak roughness difference is even more dramatic due to the poor uniformity for the InAlAs structure. The vastly improved surface morphology for the InAsP graded buffer is believed to be due to advantages of grading the mole fraction of the group-V sublattice, which neither influence growth rate nor require temperature changes for MBE growth, hence providing an extra degree of freedom compared to grading on the group-III sublattice. Detailed investigations on this comparison and reporting of device performance as a function of graded buffer type are the subjects of forthcoming publications.

In conclusion, relaxed high-quality compositionally step-graded InAs$_y$P$_{1-y}$ layers with As compositions of $y = 0.4$, corresponding to a lattice mismatch of $\sim 1.3\%$ were grown on InP substrates using solid-source MBE. Plan-view TEM revealed an average TDD of $4 \times 10^7$ cm$^{-2}$. An extremely ordered crosshatch morphology was observed with very low surface roughness compared to cation-based graded buffers with a similar mismatch on InP. Hence, MBE-grown InAs$_y$P$_{1-y}$ step-graded buffers hold great promise as a virtual substrate technology for InP-based infrared devices.

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FIG. 4. AFM images from the surface of (a) InAs$_{0.4}$P$_{0.6}$ layer grown on InP substrate using a four-step InAs$_{1-y}$P$_{y}$ layer and (b) In$_{0.7}$Al$_{0.3}$As layer grown on InP substrate using a five-step In$_{1-x}$Al$_x$As layer. The scan area and the rms roughness were 40 μm × 40 μm, 3.16 nm, and 10.53 nm, respectively. Total mismatch is 1.2% and layers are more than 80% relaxed.

\[ a_{layer} = \frac{(2C_{12}a_x + C_{11}a_y)}{(2C_{12} + C_{11})}, \]

\[ R = \frac{(a_x - a_y)}{(a_{layer} - a_x)}. \]