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Solar Energy Materials & Solar Cells 91 (2007) 908–918

Solar Energy Materials and Solar Cells

www.elsevier.com/locate/solmat

Optimization of buffer layers for lattice-mismatched epitaxy of $Ga_xIn_{1-x}As/InAs_yP_{1-y}$ double-heterostructures on InP

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Received 23 December 2006; accepted 14 February 2007
Available online 6 April 2007

Abstract

We optimize $InAs_yP_{1-y}$ buffer layers and compositional grades for lattice-mismatched heteroepitaxy of $Ga_xIn_{1-x}As/InAs_yP_{1-y}$ double-heterostructures on InP. The strains of the active and buffer layers depend on the bulk misfit difference between these layers. The misfit difference is adjusted to eliminate strain in the active layer, thus avoiding misfit dislocations and surface topography that would otherwise form to relieve strain. The optimized structure uses an "overshoot" with respect to the conventional design in the misfit and As composition of the $InAs_yP_{1-y}$ buffer. Nearly optimized heterostructures typically show excellent structural quality and extended minority-carrier lifetimes.

Keywords: Epitaxy of thin films; Semiconductors; Indium phosphide; Transmission electron microscopy; Diffraction; Chemical vapor deposition

1. Introduction

$Ga_xIn_{1-x}As$ (GaInAs) plays an established role in a variety of low-bandgap device applications, including thermophotovoltaic (TPV) power generation [1]. $InAs_yP_{1-y}$ (InAsP) is an ideal partner alloy for forming compositional grades to low-bandgap, lattice-mismatched GaInAs ($x < 0.47$) on InP, because the InAsP passivates the GaInAs surface. Exceptional device performance was reported [2] in 0.60 eV GaInAs heterostructures with InAsP grades on InP. This work identifies the influences of the grade on the structural properties of 0.52 eV GaInAs double heterostructures (DHs).

Lattice-mismatched heteroepitaxy greatly expands the number of film/substrate combinations available for semiconductor device design. For example, alloys derived from the III–V binary compounds span a range of optical bandgaps, but a particular alloy composition is likely to be lattice mismatched to a preferred binary substrate [3]. For cubic semiconductors, lattice mismatch results from the difference in the bulk lattice constant a of the film material with the substrate lattice constant a_s. This difference generates strain and/or misfit dislocations in mismatched heterostructures, which deteriorate the film quality.

The incorporation of a structural grade, usually comprising an alloy, can greatly improve the quality of lattice-mismatched active layers. The composition and misfit are varied linearly in the grade, which is then terminated with a buffer layer that provides a template for growth of the active layer. However, the biaxial stress on the buffer layer alters the lattice constant $a^{(||)}$, measured parallel to the substrate plane. Therefore, it is necessary to calibrate the in-plane strain $\varepsilon = [a^{(||)}/a]-1$ in the buffer, than to select the appropriate buffer composition that is nearly lattice-matched to the desired active layer.

The bulk misfit of a layer with respect to the substrate can be expressed in terms of the coherency

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doi:10.1016/j.solmat.2007.02.008

strain $\varepsilon_c = (a_s/a)-1$ as

$$f \equiv -\varepsilon_c = 1 - \frac{a_s}{a}. \tag{1}$$

Misfit is a useful benchmark to gauge the net deviation from the lattice-matched condition. The approximation $f \approx (a/a_s)-1$ suffices for highly mismatched films. The in-plane misfit is defined as

$$\bar{f} \equiv f + \varepsilon = \frac{a^{(\|)} - a_s}{a}. \tag{2}$$

For direct growth on a substrate, the misfit dislocation density is approximately proportional to $|\bar{f}|$, which vanishes when the interface is fully coherent.

Corrections in the misfit of the buffer layer to compensate for in-plane strain have been suggested as a means to improve material quality [4,5]. In the $Si_{1-x}Ge_x$ system, the thickness, composition, and growth parameters of partially relaxed buffer layers were used to control the strain within superlattices [6]. In GaInAs/InAsP photodetectors on InP, reductions in dark current and corresponding improvements in efficiency were obtained by adjusting the InAsP buffer composition [7] so that the bulk misfit of the buffer layer exceeded that of the active layer. This "overshoot" represents an increase Δy in the As content of the InAsP buffer layer by a few percent over the composition that is lattice-matched to bulk GaInAs.

We previously showed that the strain in InAsP buffer layers on InAsP step grades grown on InP is essentially independent of the net misfit [8], as anticipated from equilibrium theory. In this work, we calibrate the residual strain in the buffer layer and refine the conventional GaInAs/InAsP DH design scheme (in which the active and buffer layers have precisely the same bulk misfit with respect to the substrate) to compensate for the buffer strain. From empirical analysis, we predict conditions for the complete elimination of strain in the GaInAs active layer using standard growth conditions. Good interfacial coherence can be maintained across the GaInAs/InAsP interface over a relatively broad range of InAsP buffer-layer compositions. The minority-carrier lifetime τ is used as a benchmark of material quality, but is subject to a variety of influences. Finally, we discuss a general criterion and recommendations for designing uniform compositional grades on which to grow mismatched active layers.

2. Experimental procedures

This article describes detailed characterization of GaInAs/InAsP DHs grown by atmospheric-pressure metalorganic vapor-phase epitaxy. Growth was performed on 2″ Fe-doped, InP semi-insulating substrates miscut 2° from [0 0 1] to [1 0 1]. Further details of the growth are provided elsewhere [8]. The GaInAs/InAsP DHs described here each used a uniform InAsP n-step grade, where the first $n-1$ steps each have thickness $\Delta h_{\text{step}} = 0.30\,\mu\text{m}$ and the final step forms the buffer layer with misfit f_b and thickness $h_b = 1.0\,\mu\text{m}$. The target structure has a uniform misfit increment of $\Delta f_{\text{step}} = f_b/n$ in the grade, such that the misfit of step m (where $m = 1,\ldots,n$) is given by $f_m = (m/n)f_b$. The GaInAs active layers each have a thickness of $h_a = 2.0\,\mu\text{m}$ and a target bandgap of 0.52 eV ($f_a = 1.65\%$), which is typical for TPV applications. Additional InAsP grade structures were grown without the active layer over a range of buffer-layer thicknesses for strain calibration.

Transmission electron microscopy (TEM) samples were prepared in $\langle 1\,1\,0 \rangle$ cross-section by polishing, dimpling, and Ar ion milling with sector control and liquid N_2 cooling. Images were acquired using the in-plane 220 dark-field condition on a Philips CM30 operated at 300 kV.

Compositions and strain were measured by X-ray diffraction (XRD) $\theta/2\theta$ patterns on a Scintag X1 four-circle diffractometer with a solid-state detector using Cu-Kα radiation. The tilt-dependent, "strained" lattice constant $a(\Psi)$ for each layer varies linearly with $\sin^2(\Psi)$, where the angle Ψ is measured from the substrate normal [8]. This procedure requires iterative refinement of the sample orientation, particularly about the ω-axis, for each layer, to eliminate deviations in the radial peak positions due to strain, misorientation, or both. The peak position is then equivalent to that measured in two-dimensional reciprocal-space maps. Least-squares fits of the K-α doublets are made to Pearson-7 line shapes. Elastic coefficients are linearly interpolated from the end-point values.

Ultrahigh-frequency photoconductivity decay (PCD) was used to measure the minority-carrier lifetime τ of GaInAs/InAsP DHs [9]. Photoluminescence (PL) spectra were acquired by Fourier-transform spectroscopy. Mechanical dimpling and Br:methanol etching were used for PL depth profiling.

3. Results and discussion

We now focus on structural optimization of GaInAs/InAsP DHs. A series of DHs grown over a range of buffer compositions with approximately fixed GaInAs composition are characterized. These results are used to formulate empirical optimization criteria for GaInAs/InAsP DHs. We outline a general approach to structural optimization by varying the composition profile within the step grade.

3.1. Microstructure of GaInAs/InAsP DHs

Analysis of GaInAs/InAsP DHs was performed in TEM cross-section to reveal the dislocation distribution and morphology in the active region (Fig. 1). In a particular sample set, the number of steps n in the grade was varied, with the composition increment in the grade held constant, so that the last step comprised a buffer with the desired composition (Table 1). In the conventional DH structure ($n = 8$), the target, bulk lattice mismatch of the buffer layer is equal to that of the active layer. The degree of interfacial coherence between the film and buffer in each sample is qualitatively apparent from the density of resident misfit