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III-V Growth on Silicon Toward a Multijunction Cell

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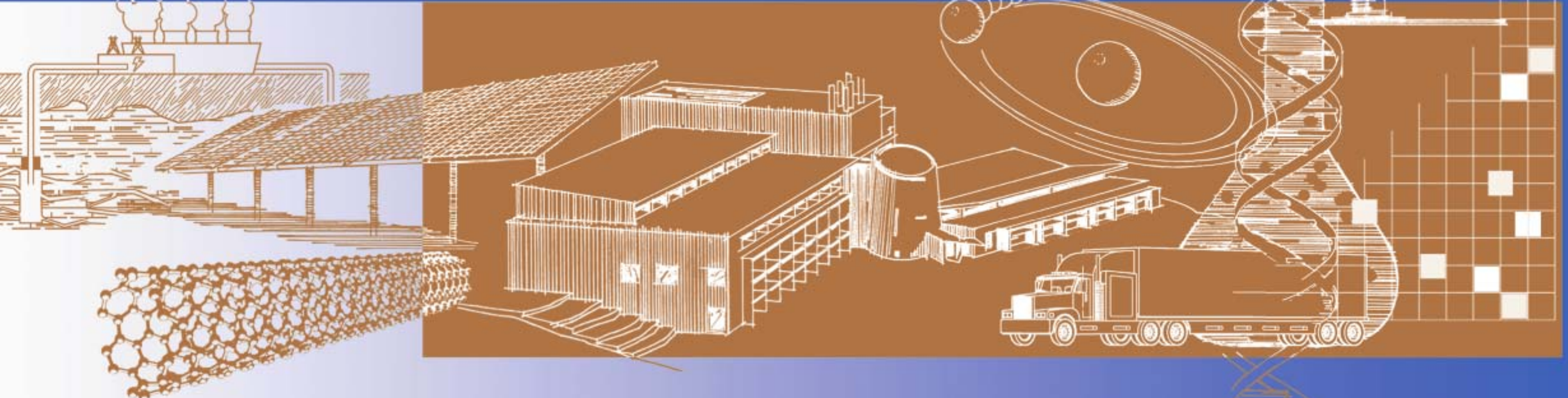

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ABSTRACT

A III-V on Si multijunction solar cell promises high efficiency at relatively low cost. The challenges to epitaxial growth of high-quality III-Vs on Si, though, are extensive. Lattice-matched (LM) dilute-nitride GaNPAs solar cells have been grown on Si, but their performance is limited by defects related to the nitrogen. Advances in the growth of lattice-mismatched (LMM) materials make more traditional III-Vs, such as GaInP and GaAsP, very attractive for use in multijunction solar cells on silicon.

1. Objectives

Today's fast-growing photovoltaic industry relies on silicon. Although the efficiencies of silicon modules have slowly increased, a two-junction cell on silicon has the potential for a dramatic (>10% absolute) efficiency boost. The purpose of this project is to explore the potential for low-cost, high-efficiency III-V-on-silicon solar cells.

2. Technical Approach

2.1 Nucleation of GaP Growth on Si

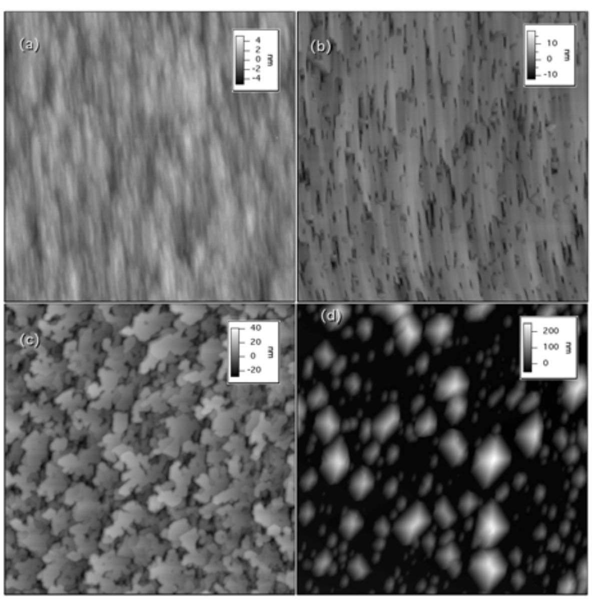

Fig. 1. AFM images of nominally 20-40nm GaP layer grown on Si. (a) PC197:APD-free [0.8nm RMS], (b) PC195:smooth, but some APDs [2.3nm RMS], (c) MG024:step-bunched terrace growth [7.9nm RMS], (d) MG025:island growth [52nm RMS]. All images are 5 x 5 µm and roughness is indicated in brackets.

The growth of an initial layer of smooth single-domain III-V layer on Si is an important step to achieve high-quality III-V materials grown on Si. We have studied a wide range of growth parameters to optimize this step. Atomic force microscopy (AFM), x-ray diffraction (XRD), transmission electron microscopy (TEM), and spectroscopic ellipsometry (SE) are used to measure and characterize these thin layers of GaP on Si.

2.2 Low dislocation density GaAsP and GaInP

LM dilute-nitride GaNPAs materials grown on Si[1,2] or GaP[3] have short diffusion lengths that limit the performance of such junctions. This is due to nitrogen related defects. GaAsP and GaInP materials are LMM with Si, but do not possess the detrimental nitrogen-related defect. Step graded buffer layers are grown to relieve the strain inherent to LMM heteroepitaxial growth. Growth conditions and layer structures are optimized to reduce the threading dislocations that are also detrimental to the diffusion lengths of these materials. The threading dislocations are imaged using spectral cathodoluminescence (CL) and TEM, and the resulting electrical properties are characterized with quantum efficiency (QE) of an electrochemical junction.

3. Results and Accomplishments

3.1 Nucleation of GaP growth on Si

We have employed state-of-the-art analytical techniques to understand the surface of the silicon and subsequent nucleation of GaP within a metal-organic chemical vapor deposition (MOCVD) reactor.[4,5] We find that by growing on silicon substrates miscut 2° from (001) toward (111), we can achieve antiphase domain (APD)-free layers of GaP with extremely low roughness. Figure 1 shows AFM images of various GaP-on-Si layers. Oxide-free Si surfaces at growth temperature are required for APD-free growth. These can be achieved by desorbing the oxide at >1000°C under H_2 or in-situ etching with AsH_3 pretreatment at <800°C. Extremely high PH_3/Ga ratios are required during the initial nucleation growth. The temperature and pressure during growth are also key parameters. APD densities increase with reactor pressure making it very difficult to grow completely APD-free GaP-on-Si in our atmospheric-pressure reactor.

The high crystalline quality and low interface roughness of these GaP-on-Si layers have been

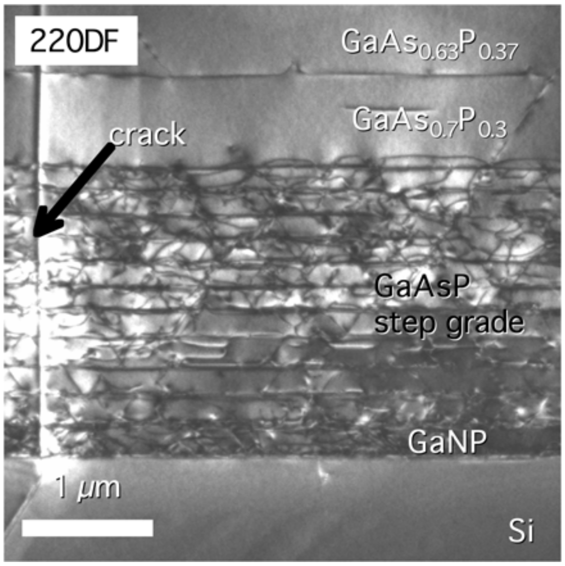

Fig. 2. Cross-sectional TEM of LMM GaAsP-on-Si graded structure (MF815).

demonstrated by nearly perfect dynamical fits to XRD measurements.

3.2 Low dislocation density GaAsP and GaInP

The dislocation density (DD) in thick layers of LMM GaAsP and GaInP is reduced by step graded buffer layers. Figure 2 shows TEM of a step-graded structure. Nearly LM GaNP layers are also used to achieve small steps in the mismatch of the grade. GaInP compositions are much easier to control, but GaAsP grades offer smoother morphology. The composition and strain state of the layers in these complex structures can be analyzed ex-situ using XRD reciprocal space maps as shown in Fig. 3. The management of strain during growth is difficult to deduce as a significant difference in thermal expansion between III-V materials and Si results in large changes during cool-down. Cracking of the

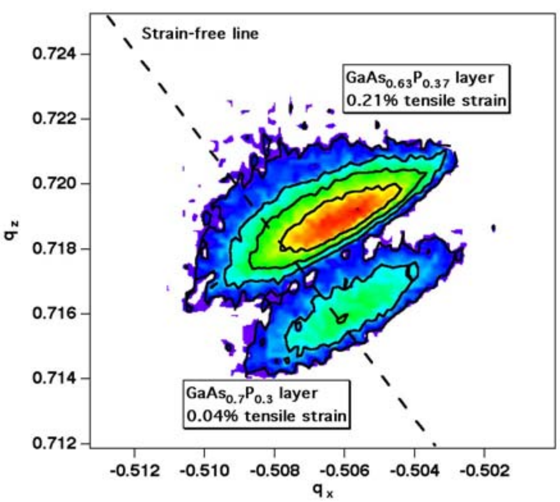

Fig. 3. X-ray diffraction reciprocal space map of the top layers of the LMM structure shown in Fig. 2. Grazing incidence 224 reflection.

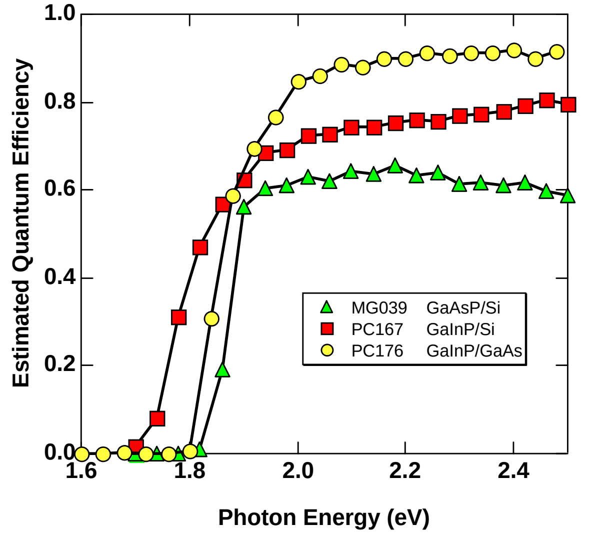

Fig. 4. Electrochemical QE of LMM III-V grown on Si compared with GaInP grown on GaAs.

structures due to large tensile strains during cool-down can be avoided by maintaining a residual compressive strain during growth. CL images reveal threading dislocation densities of about $8x10^{7}$ cm^{-2} for unoptimized step-graded structures on Si. The electrochemical QE of step-graded GaAsP and GaInP structures in Fig. 4 show estimated quantum efficiencies approaching those of high quality GaInP grown on GaAs. The electrochemical QEs for these LMM materials on Si need to be confirmed in solid-state solar cells.

4. Conclusions

We have demonstrated nucleation of thin layers of high quality GaP on silicon. Subsequent growth of graded layers to relieve strain in LMM III-V materials has resulted in III-V layers with dislocation densities in the mid 10^{7} cm^{-2}. Further reduction in the dislocation density should make possible high-efficiency III-V on silicon multijunction solar cells.

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