Relaxed GaP on Si with low threading dislocation density

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Epitaxial growth of 1.7 eV $GaAs_{0.75}P_{0.25}$ on GaP/Si templates offers a promising path to low-cost, high-efficiency tandem solar cells. While nucleation of thin, strained GaP on Si without anti-phase domains and stacking faults is now well established, the relaxation process of GaP on Si remains poorly understood. Threading dislocation densities (TDD) > 10^7 cm^{-2} in relaxed GaP on Si have been observed, despite the small lattice mismatch of ~0.45%. Our prior work revealed that the TDD of relaxed GaP on Si is dominated by dislocation glide at low temperatures (e.g. < 505°C) and by dislocation nucleation at high temperatures (e.g. > 575°C), with lowest TDD of 1.7×10^6 cm^{-2} [1]. We also showed that the TDD of the relaxed GaP layer strongly influences the TDD and efficiency of the $GaAs_{0.75}P_{0.25}$ active region, which emphasizes the importance of controlling the initial relaxation.

Here, we describe a two-step MBE growth process to suppress heterogeneous dislocation nucleation and improve dislocation glide during relaxation of GaP on Si. Initiating growth with a thin, low-T layer and subsequently growing a high-T layer for a combined thickness of ~0.5 μm enabled TDD reduction to 1.0×10^6 cm^{-2} in relaxed GaP on Si, which is the lowest value to date. We will show that the low-T step strongly suppresses dislocation nucleation, while the high-T step improves dislocation glide and surface morphology. This reduction in GaP TDD is expected to enable TDD values of $2\text{-}3\times10^6$ cm^{-2} for $GaAs_{0.75}P_{0.25}$ solar cells on GaP/Si along with substantial efficiency improvements over current state-of-the-art.

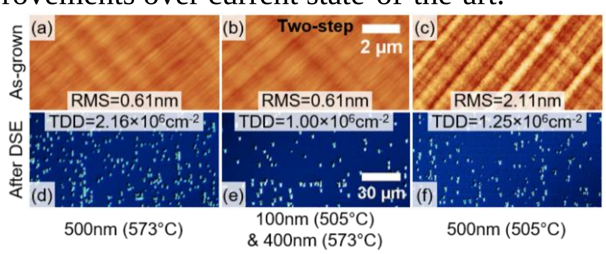

Figure 1. Two-step growth improvement (center) over single-step growths. (a-c) AFM image (z-range = 0-17.8 nm) of as-grown surfaces. (d-f) Nomarski micrographs after defect-selective etching.

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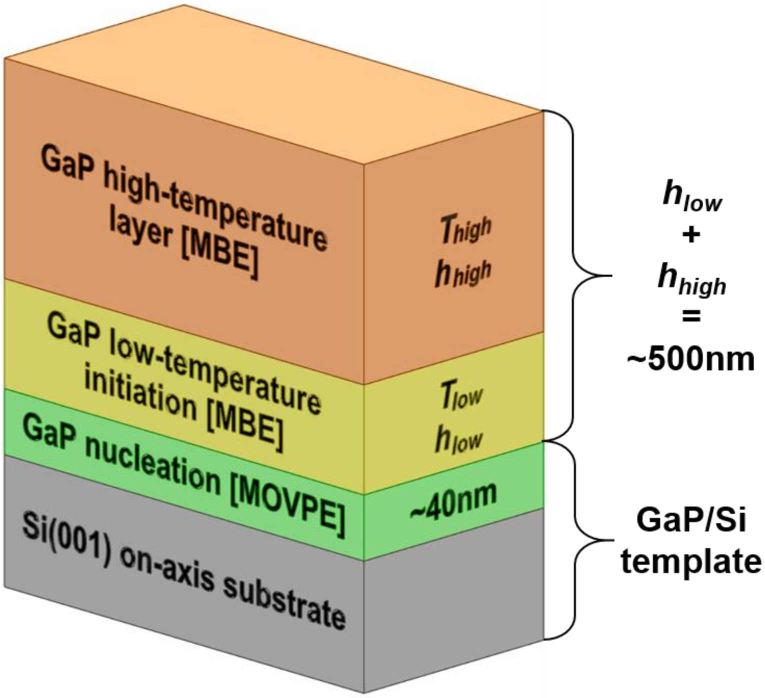

Figure 2. Layer structure of two-step GaP growth on GaP/Si templates. As-received GaP/Si templates have a ~40 nm GaP nucleation layer grown by metalorganic vapor phase epitaxy (MOVPE). Growth performed by solid-source molecular beam epitaxy (MBE): first a low-temperature, T_{low}, initiation layer of thickness, h_{low}, and then a high-temperature, T_{high}, layer of thickness, h_{high}. Total MBE-grown thickness is ~500 nm.

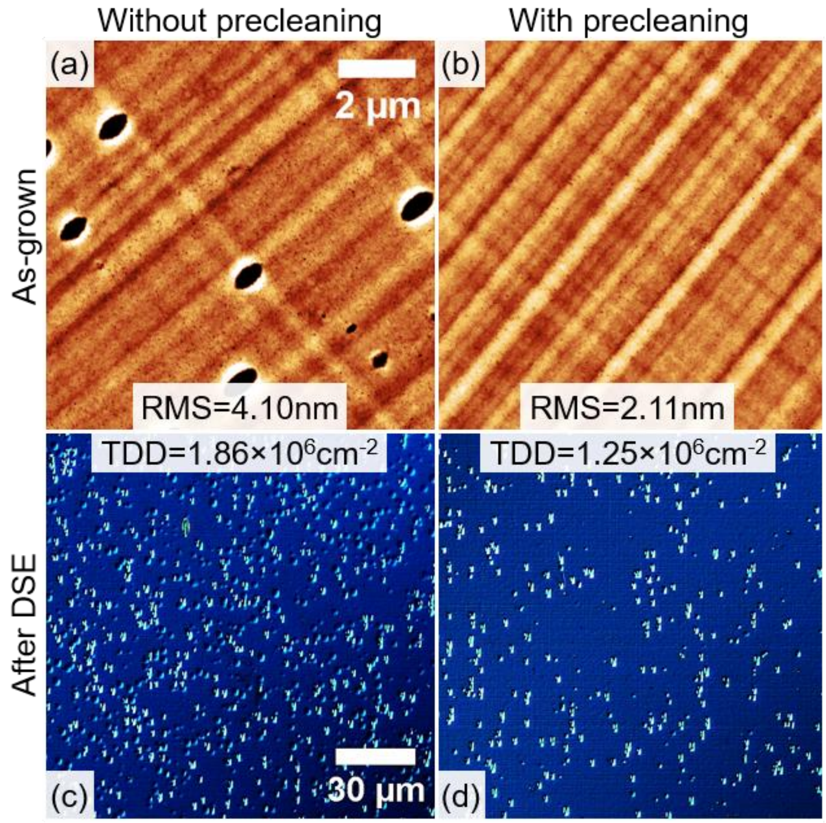

Figure 3. Comparison of GaP grown on (a,c) GaP/Si templates without precleaning and (b,d) templates with dilute aqua regia precleaning. Both samples were co-grown with single-step at 505°C. (a-b) Representative AFM images of as-grown surface morphology (z-range = 0-17.8 nm). Note pits for (a) extend lower than z-range with depth up to ~60 nm. (c-d) Representative Nomarski micrographs after defect selective etching (DSE). Precleaning of as-received GaP/Si templates lowered GaP TDD and improved as-grown surface morphology by reducing pitting, suggesting removal of heterogeneous dislocation nucleation sites.

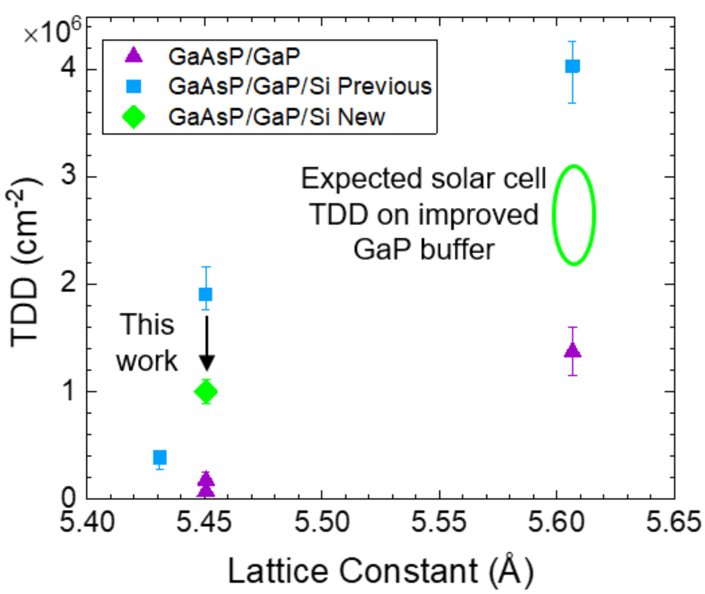

Figure 4. Evolution of TDD for growth on GaP/Si (blue, green) from template to final device as a function of relaxed lattice constant. Growth on bulk GaP (purple) also shown from substrate to device. Each is represented at the relaxed lattice constant (except for the nearly pseudomorphic GaP/Si template). TDD for GaP substrate and relaxed GaP determined by DSE; TDD for as-received GaP/Si template estimated using electron channeling contrast imaging. TDD of ~1.7 eV GaAsP (5.61Å) determined by electron beam-induced current. Error bars show range of measurements from multiple images.

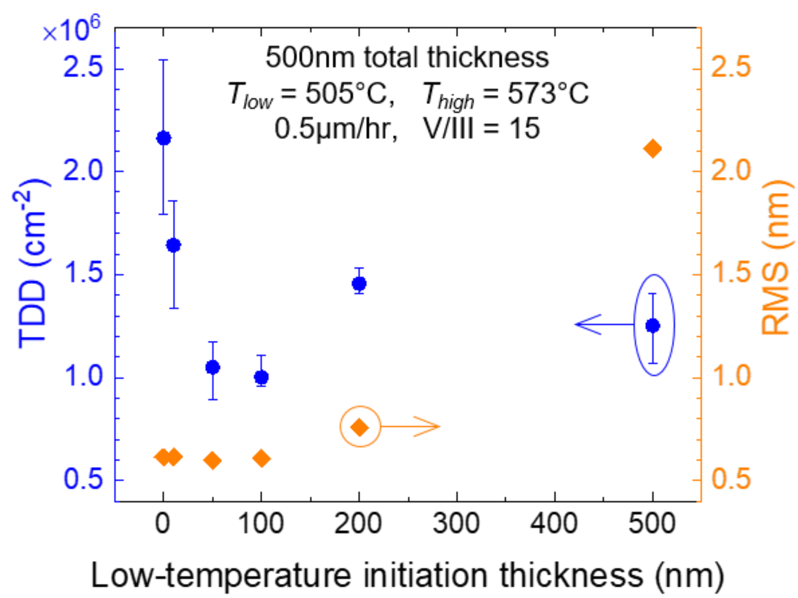

Figure 5. TDD and RMS roughness for relaxed GaP on GaP/Si as a function of low-temperature initiation layer thickness, h_{low}. Growth conditions are inset. All samples grown to ~500 nm of total MBE GaP thickness. Samples with h_{low} = 0 nm and h_{low} = 500 nm are single-step growths at 573°C and 505°C, respectively. RMS determined from 10×10 µm² AFM images.

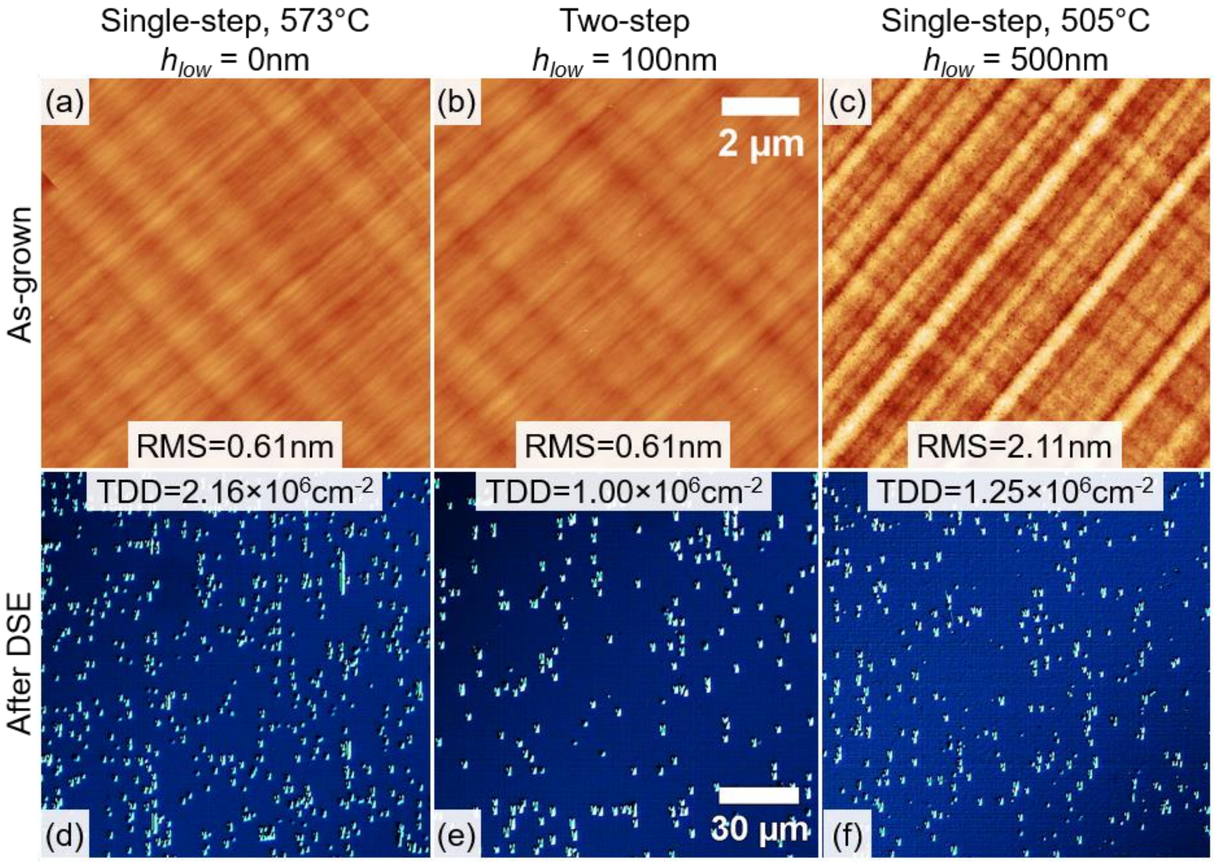

Figure 6. Expanded AFM images and Nomarski micrographs of Fig. 1 (main abstract page).

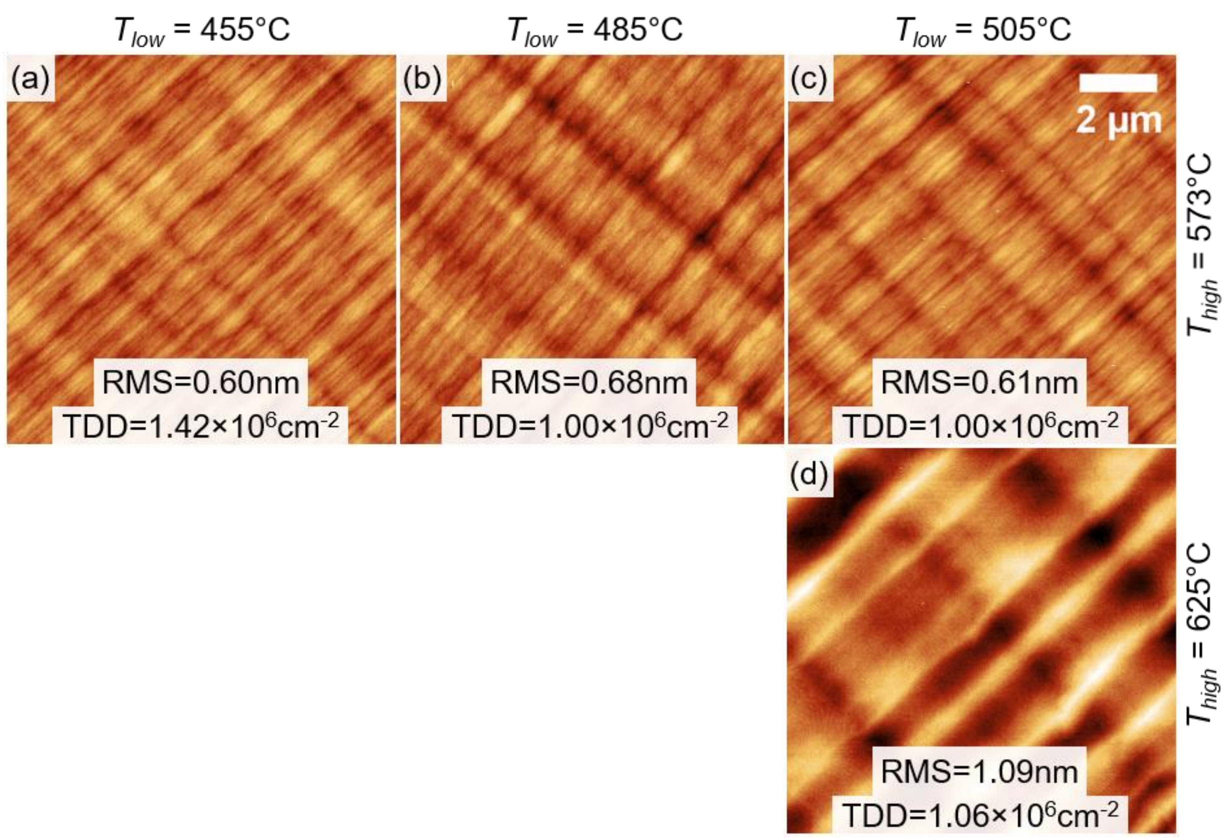

Figure 7. Comparison of surface morphologies for two-step growths with varied T_{low} and T_{high} (z-range = 0-6.33 nm). (a-c) Show varied T_{low} causes little surface morphology change, but increased TDD at T_{low} = 455°C. (c-d) Show varied T_{high} results in little TDD change, but major surface morphology changes. Monolayer steps observed in (d) indicate change to step-flow growth for 625°C growth. In conventional single-step growth at 625°C, TDD of ~4×10^6 cm^{-2} is expected [1], which is ~4× higher than for two-step growth.