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Effectiveness of Low Temperature Growth for Low Dislocation Density in III-V on Si Towards High-Efficiency III-V/Si Tandem Solar Cells

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Abstract

Si tandem solar cells are expected to have great potential of terrestrial and new market application because of high efficiency, light weight and low cost potential. This paper focusses on III-V/Si tandem solar cells grown directly on Si. This paper presents analytical results for effectiveness of low temperature growth of III-V layer on Si for realizing low dislocation density. Low dislocation density of less than 3x10^5 cm^{-2} in GaAs on Si by low temperature growth is demonstrated.

1. Introduction

Although 37.9% efficiency has been realized with InGaP/InGaAs/Ge 3-junction solar cells, III-V compound multi-junction solar cells are still expensive. The Si tandem solar cells [1] are very attractive for realizing super high-efficiency and low cost. This paper focusses on direct growth of III-V/Si tandem cells on Si. However, one of major problems for III-V/Si system is to realize low dislocation density.

This paper presents effectiveness of low temperature growth of III-V layer on Si substrates for realizing low density dislocations on Si substrates. An approach for low temperature growth of GaAs thin films on Si substrates is shown.

2. Discussion about mechanism for dislocation density reduction in III-V compounds on Si by low temperature growth

The major problems in growing high quality III-V compound semiconductor films on Si are lattice mismatch and residual stress caused by difference of thermal expansion coefficient between III-V compound film and Si substrate. Our previous results for X-ray diffraction and photoluminescence peak shift measurements [2] have shown that residual stains in GaAs and InP layers on Si are dominated by thermally induced strains after the growth. This result suggest effectiveness of low temperature growth of III-V on Si for reducing dislocation density.

The thermally induced strain ε_{th} is expressed by

$\varepsilon_{th} = \Delta T \Delta\alpha$, (1)

where ΔT is temperature difference between growth and room temperature and $\Delta\alpha$ is thermal expansion coefficient difference between III-V compound film and Si substrate. Figure 1 shows thermally-induced strains estimated from eq. (1) in films after growth and residual stains measured by X-ray diffraction and photoluminescence for GaAs, GaP and InP films as a function of temperature. The smaller residual strains than the $\Delta T\Delta\alpha$ value shown in Fig. 1 suggests that strain relaxation occurs during cooling process after growth. It is shown in Fig. 1 that strain is thermally induced as temperature decreases after growth and dislocations can be easily generated under high stress condition. As shown in Fig. 1, the freezing temperature T_f for dislocation reconfiguration estimated from remained strains are 450 ^{0}C ± 90 ^{0}C for GaAs/Si. Therefore, low temperature growth of less than freezing temperature is thought to be very effective for realizing low dislocation density in III-V compound films on Si substrates.

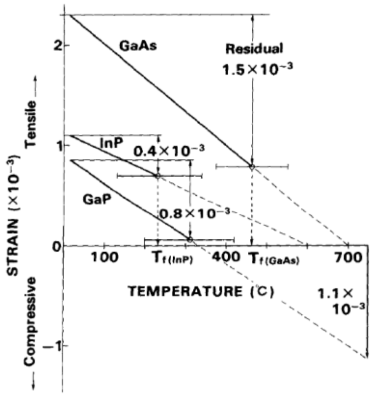

Fig. 1 Thermally-induced strains estimated from eq. (1) in films after growth and residual stains measured by X-ray diffraction and photoluminescence for GaAs, GaP and InP films as a function of temperature.

Thermally induced strain σ_{th} is expressed by

$\sigma_{th} = H\varepsilon_{th}$, (2)

where H is Young's modulus and is 83 GPa in the case of GaAs. Using eqs. (1) and (2), growth temperature dependence of strain σ_{th} is estimated. It is known in bulk GaAs crystals that dislocations are generated at high stress condition of larger than critical stress [3]. The critical stress for dislocation generation depends on the temperature stressing. The yield stress $\sigma_{un\text{-}doped}$ in un-doped GaAs crystals and the yield stress σ_{doped} in doped GaAs crystals reported by Yonenaga et al. [3] are given by

$\sigma_{un\text{-}doped}$ [MPa] = 0.004exp[0.46 eV/kT] , (3)

σ_{doped} [MPa] = 0.0019exp[0.63 eV/kT] , (4)

where k is Boltzmann constant and T is absolute temperature.

Figure 2 shows calculated growth temperature dependence of thermally induced stress σ_{th} for GaAs on Si and the yield stress $\sigma_{un\text{-}doped}$ in the case of un-doped and the yield stress σ_{doped} in the case of doped GaAs. If thermal stress σ_{th} is larger than the yield stress $\sigma_{un\text{-}doped}$ or the yield stress σ_{doped}, thermally-induced dislocations are thought to be generated by thermally-induced stress. From Fig. 2, freezing temperatures T_f estimated from the yield stress in the case of un-doped and doped GaAs are 210 ^{0}C and 440 ^{0}C, respectively. Heteroepitaxial growth of GaAs-on-Si with low temperature of less than 210 - 440 ^{0}C is thought to be very effective for realizing low density of dislocations in GaAs on Si.

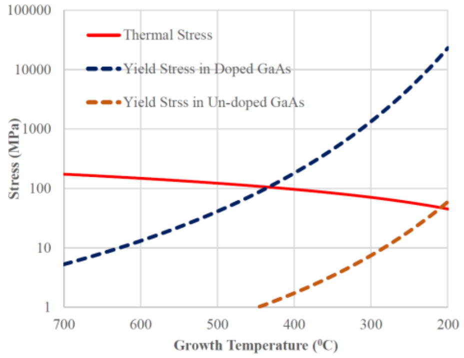

Fig. 2 Calculated growth temperature dependence of thermally induced stress for GaAs on Si and yield stress in un-doped and doped bulk GaAs crystals.

3. Preliminary results for low dislocation density in GaAs grown directly on Si by low temperature growth

The authors have tried the standard 2 step growth of low temperature (230 ^{0}C) and high temperature growth (600 ^{0}C) by MBE (molecular beam epitaxy) growth and our 2 step growth of low temperature (230-280 ^{0}C) and high temperature growth (300-570 ^{0}C) by MEE (migration-enhanced epitaxy). Molten KOH etching was carried out to estimate the dislocation density and observe the dislocation behavior in the GaAs films grown directly on Si. The KOH etching was carried out at 300-350 °C and the observed small etch pits were also counted as etch pit density (EPD). As shown in Table1, low dislocation density of less than $3\text{x}10^5$ cm^{-2} in GaAs-on-Si by low temperature growth has been demonstrated.

Table 1 Comparison of dislocation density in GaAs grown directly on Si

Growth condition	EPD(cm^{-2})
2 step growth by standard MBE(600°C/280°C)	5×10^7- 2.2×10^8
2 step growth by MEE (570°C(2.1μm)/280°C(70nm))	3×10^5
2step growth MEE (300°C(1.5μm)/280°C (70nm)	1×10^4

4. Analysis of efficiency potential of III-V/Si tandem cells

We introduce an analytical model [3] for comparing the sources of efficiency loss of different types of solar cells. This model only attributes the efficiency loss to non-radiative recombination loss and resistance loss, which is a reasonable assumption because conventional solar cells often have a minimal optical loss. The non-radiative recombination loss is quantified by external radiative efficiency (ERE), which is the ratio of radiatively recombined carriers against all recombined carriers. In this work, we estimate the EREs of various solar cells by the following relation [1]:

$V_{oc} = V_{oc:rad} + (kT/q)\ln(ERE)$, (5)

where V_{oc} is the measured open-circuit voltage, k is Boltzmann constant, T is the absolute temperature, and q is the elementary charge. $V_{oc:rad}$ is the radiative open-circuit voltage. Previously, the authors have shown effects of dislocations upon minority-carrier lifetime by considering one dimensional transport of minority carriers to dislocations [1]. The resulting dislocation-limited minority-carrier lifetime τ_d is given by

$1/\tau_d = \pi^3 N_d D/4$, (6)

where N_d is dislocation density, and D is minority-carrier diffusion constant. Therefore, the effective minority-carrier lifetime τ_{eff} is expressed by the following equation:

$1/\tau_{eff} = 1/\tau_{rad} + 1/\tau_d = BN + \pi^3 N_d D/4$, (7)

where, τ_{rad} is minority-carrier lifetime for radiative recombination, B is the radiative recombination probability, and N is the carrier concentration. For GaAs, B value is 2 x 10^{-10} cm^3/s.

Figure 3 shows calculated 1-sun efficiencies of GaAs single-junction, III-V/Si 2-junction and 3-junction solar cells estimated from dislocation density dependence of minority-carried lifetime by using eqs. (5)-.(7) in comparison with current efficiencies [1] of GaAs single-junction, III-V 2-junction and 3-junction solar cells grown directly on Si as a function of dislocation density. Low dislocation density with dislocation densities of less than $3\text{x}10^5$ cm^{-2} obtained in this study is thought to be very attractive for realizing high efficiency III-V/Si 2-junction and 3-junction solar cells that have efficiency potential of 33% and 38%, respectively, as shown in Fig. 3.

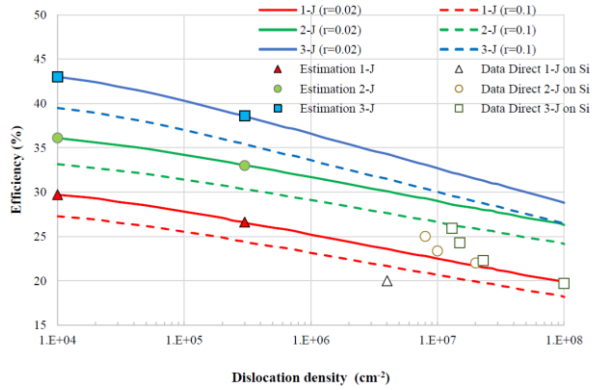

Fig. 3 Calculated 1-sun efficiencies of GaAs single-junction, III-V/Si 2-junction and 3-junction solar cells estimated from dislocation density dependence of minority-carried lifetime by using eqs. (5)-(7) in comparison with those current efficiencies as a function of dislocation density.

5. Summary

The Si tandem solar cells are expected to have great potential of terrestrial and new market application because of high efficiency, light weight and low cost potential. This paper focused on III-V/Si tandem solar cells grown directly on Si and presented analytical results for effectiveness of low temperature growth of III-V on for realizing low dislocation density. Low dislocation density of less than $3\text{x}10^5$ cm^{-2} in GaAs-on-Si by low temperature growth was demonstrated. Such a low dislocation density shows high efficiency potential of 33% and 38% for III-V/Si 2-junction and 3-junction tandem solar cells, based on our analytical results.

References

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