Efficiency calculations of thin-film GaAs solar cells on Si substrates

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Dislocation effect upon the efficiency of single-crystal thin-film AlGaAs-GaAs heteroface solar cells on Si substrates is analyzed. Solar-cell properties are calculated based on a simple model; in the model, dislocations act as recombination centers to reduce the minority-carrier diffusion length in each layer and increase the space-charge layer recombination current. Numerical analysis is also carried out to optimize thin-film AlGaAs-GaAs heteroface solar-cell structures. The fabrication of thin-film AlGaAs-GaAs heteroface solar cells with a practical efficiency larger than 18% on Si substrates appears possible if the dislocation density in the thin-film GaAs layer is less than 10^6 cm^{-2}.

I. INTRODUCTION

It is well known that GaAs has great potential for space and terrestrial photovoltaic device applications. Although high-efficiency GaAs solar cells have been obtained on GaAs[1] and Ge substrates,[2] they have thus far proved much too costly for large-scale space and terrestrial applications.

A new approach has been proposed for realizing high efficiency, low cost, and light weight GaAs cells.[3,4] This method utilizes single-crystal GaAs films deposited on low cost Si substrates. However, successful development of thin-film GaAs solar cells with 15% or greater efficiency has not been made to date. This is because it is more difficult to grow a high-quality GaAs epitaxial layer on a Si substrate because of a large lattice mismatch of about 4%. The harmful effect of dislocations on GaAs solar-cell electrical properties must be considered. Although antiphase domain boundaries in GaAs are also expected to act as recombination centers, single domain GaAs layers can be grown by optimizing substrate surface treatment and heteroepitaxial growth conditions. Therefore, in order to realize high efficiency thin-film GaAs solar cells, it is important to clarify the effects of dislocations upon the electrical and photovoltaic properties of GaAs. Moreover, there has been no report that considers the effect of dislocations on thin-film GaAs cells and deals with their efficiency calculations.

In this paper, correlations between minority-carrier diffusion lengths and dislocation density have been analyzed. In addition, solar-cell parameters for thin-film AlGaAs-GaAs heteroface solar cells shown in Fig. 1 are calculated based on their relationships. It is estimated that one could fabricate thin-film AlGaAs-GaAs heteroface solar cells with an efficiency of 18% or greater on Si substrates if the dislocation density is less than 10^6 cm^{-2}.

A numerical analysis has been carried out to obtain curves relating cell efficiency for thin-film AlGaAs-GaAs heteroface cells to junction depth and other cell physical parameters.

II. MINORITY-CARRIER DIFFUSION LENGTH ESTIMATION

A. Effect of dislocation density on diffusion length

Dislocations play a dominant role in determining the electrical and photovoltaic properties of thin-film GaAs solar cells. They act as recombination centers in the same manner as impurities and other defects. The recombination loss at dislocations which reduces the short-circuit current and increases the excess leakage current is thought to be the predominant loss mechanism in thin-film GaAs solar cells. Dislocation recombination centers reduce the minority-carrier lifetime and diffusion length. Minority-carrier diffusion length is given by

$$1/L^2 = 1/L_0^2 + 1/L_d^2 + 1/L_I^2, \tag{1}$$

where L_d, L_I, and L_0 are diffusion lengths associated with minority-carrier recombination with a majority carrier at a dislocation, at an impurity and at other unknown defects, respectively.

The dislocations were assumed to be uniformly distributed in GaAs and model calculations were done to obtain diffusion length versus dislocation density relationships. The diffusion-limited minority-carrier diffusion length for recombination on dislocations is obtained by solving the one-dimensional continuity equation for the transport of minority carriers to the dislocations

$$\frac{\partial n}{\partial t} = \frac{D\partial^2 n}{\partial x^2}, \tag{2}$$

where n is the excess minority-carrier concentration and D is the minority-carrier diffusion coefficient. The boundary conditions are given by

$$n = 0, \quad \text{at } x = 0, \tag{3}$$

$$n/t = 0, \quad \text{at } x = x_c = 1/(\pi N_d)^{1/2}, \tag{4}$$

where x_c is the unit cell radius and N_d is the dislocation density. The resulting solution of the dislocation-limited minority-carrier diffusion length is expressed by

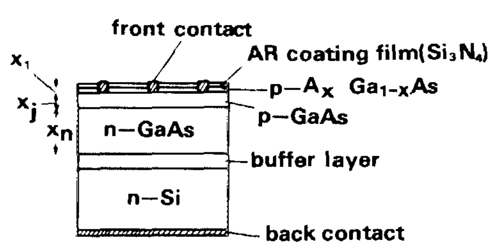

FIG. 1. Schematic diagram of a thin-film p^+-p-n AlGaAs-GaAs heteroface solar cell on a Si substrate.

$$1/L_d^2 = \pi^3 N_d/4 . \quad (5)$$

Thus, by ignoring the impurity-limited recombination, the effective minority-carrier diffusion length is derived from Eqs. (1) and (5), as follows

$$1/L^2 = 1/L_0^2 + \pi^3 N_d/4 . \quad (6)$$

The validity of this model is substantiated by the relationship between the luminescent efficiency and the dislocation density in the GaAs light emitting diodes as follows

$$\eta/\eta_0 = L^2/L_0^2 = 1/(1 + L_0^2 \pi^3 N_d/4) . \quad (7)$$

where η_0 and η are the luminescent efficiencies for the GaAs LEDs without and with dislocations, respectively.

Figure 2 shows the electroluminescent efficiency from Roedel *et al.*[5] versus the dislocation density of the GaAs light emitting diodes. Good agreement between the model calculation by Eq. (7) shown in the dashed curve and the experimental values (black dots) were obtained. This fact seems to justify the basis of the present model calculations. It has, therefore, been found that the minority-carrier diffusion length in GaAs is affected by dislocations which act as recombination centers.

It is also estimated that carrier mobility is affected by dislocation density as follows[6]

$$\mu_d = (32kT\hbar/3\pi E^2\lambda^2)[(1-v)/(1-2v)]^2(q/m^* N_d) , \quad (8)$$

where k is the Boltzmann constant, T the absolute temperature, $2\pi\hbar$ the Planck constant, v the Poisson ratio, q the electronic charge, E the deformation potential constant, m^* the effective mass of the carrier, and λ the unit crystallographic slip distance. However, in a dislocation density range of less than 10^8 cm^{-2}, the effect of decreasing mobility as the dislocation density increases is actually small, relative to the effect of decreasing carrier diffusion length, and the effect of mobility on photovoltaic properties will be small. Thus, we did not consider any change in mobility as a function of dislocation density and assumed that the change in diffusion length was the more dominant factor in determining solar-cell properties.

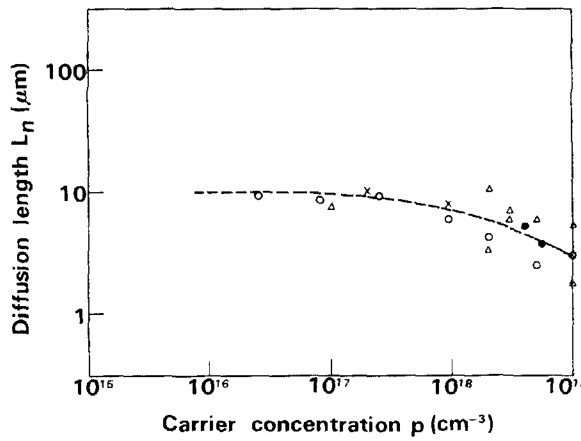

FIG. 3. An empirical fit to the electron diffusion length data in p-GaAs from Casey *et al.*[7] (circles) and Hovel[9] (triangles). The dashed line shows the empirical fitting curve.

B. Effect of impurity concentration on diffusion length

The impurity concentration affects carrier diffusion length and the diffusion coefficient in thin-film GaAs layers on Si. Figure 3 shows changes in reported values of electron diffusion length L_n as a function of carrier concentration p in p-GaAs crystals. Figure 4 shows hole diffusion length L_p dependence on carrier concentration n in n-GaAs samples. The results plotted in Figs. 3 and 4 are data reported by Casey *et al.*,[7] Sekela *et al.*,[8] and Hovel.[9] In these figures, the dashed lines show empirical fitting curves. The empirical laws for the minority-carrier diffusion legnth L (cm) dependence on carrier concentration p, n (cm^{-3}) in GaAs are expressed by

$$1/L_n^2 = 1/L_{n0}^2 + 1/L_{n1}^2 = 1/(10\times 10^{-4})^2 + 1\times 10^{-12}p , \quad (9)$$

$$1/L_p^2 = 1/(6\times 10^{-4})^2 + 3\times 10^{-11}n, \quad n \leqslant 2\times 10^{18}\ \text{cm}^{-3} , \quad (10)$$

$$L_p = 1.61\times 10^4/n^{0.443}, \quad n > 2\times 10^{18}\ \text{cm}^{-3} . \quad (11)$$

In n-GaAs, the hole diffusion length rapidly decreases with

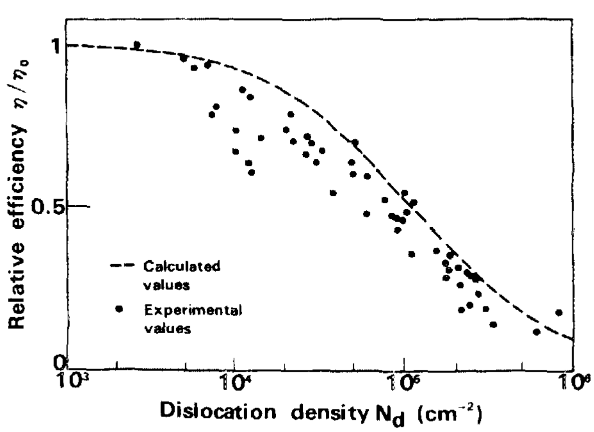

FIG. 2. Electroluminescent efficiency (black dots) from Roedel *et al.*[5] vs dislocation density for the GaAs light emitting diodes. The dashed line shows the calculated values based on the form $\eta/\eta_0 = 1(1 + L_0^2\pi^3 N_d/4)$.

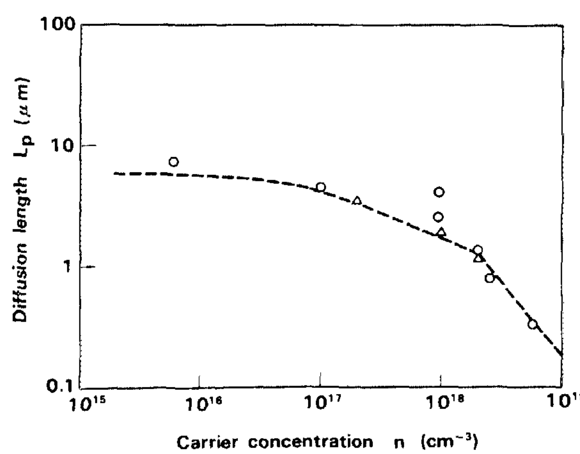

FIG. 4. An empirical fit to the hole diffusion length data in n-GaAs from Casey *et al.*[7] (open circles), Sekela *et al.*[8] (closed circles and crosses), and Hovel[9] (triangles). The dashed line shows the empirical fitting curve.

an increase in carrier concentration larger than 2×10^{18} cm^{-3}. This is because of increase in both the nonradiative recombination and Auger recombination.

The empirical laws for the minority-carrier diffusion coefficient D (cm^2/s) and majority-carrier mobility μ ($cm^2/V\ s$) dependence on carrier concentrations p, n (cm^{-3}) in GaAs were assumed in the same way as the minority-carrier diffusion length dependence on carrier concentration in GaAs as follows[10]:

$$D_n = 1.232\times10^8/(5.793\times10^5 + p^{1/3}), \quad (12)$$

$$D_p = 7.347\times10^6/(6.697\times10^5 + n^{1/3}), \quad (13)$$

$$\mu_n = 4.765\times10^9/(5.793\times10^5 + n^{1/3}). \quad (14)$$

$$\mu_p = 2.842\times10^8/(6.697\times10^5 + p^{1/3}). \quad (15)$$

III. NUMERICAL ANALYSIS TECHNIQUE OF CELL EFFICIENCY

Having derived relationships indicating how diffusion length varies as a function of dislocation density, we can postulate a general theory concerning thin-film AlGaAs-GaAs heteroface solar cells on Si substrates.

The heteroface cell structure on the Si substrate analyzed is shown in Fig. 1. x_1 is the $Al_xGa_{1-x}As$ window layer thickness, x_j is the junction depth, and x_n is the n-GaAs layer thickness. The same carrier concentration p is assumed in the p-$Al_xGa_{1-x}As$ and p-GaAs layers. The short-circuit current density J_{sc} is related to the minority-carrier diffusion lengths in the p-AlGaAs window layer, the p-GaAs layer, and n-GaAs layer, and also comes from the depletion layer.

$$J_{sc} = J_{n1}(L_{n1}) + J_{n2}(L_{n2}) + J_D(W) + J_p(L_p), \quad (16)$$

where the electron diffusion length L_{n1} in the p-AlGaAs window layer is assumed to be half of that of L_{n2} in the p-GaAs layer, according to the experimental data[11] for an AlGaAs-GaAs heteroface cell. In addition, the electron diffusion length L_{n2} in the p-GaAs and the hole diffusion length L_p in the n-GaAs are expressed by modifying Eqs. (1), (6), (9), and (10) as follows:

$$1/L_{n2}^2 = 1/(10\times10^{-4})^2 + 1\times10^{-12}p + \pi^3 N_d/4, \quad (17)$$

$$1/L_p^2 = 1/(6\times10^{-4})^2 + 3\times10^{-11}n + \pi^3 N_d/4. \quad (18)$$

The open-circuit voltage V_{oc} is given by

$$V_{oc} = (2kT/q)\ln(J_{sc}/J_{0r} + 1). \quad (19)$$

For the thin-film GaAs heteroface solar cells, the recombination current component J_{0r} is assumed to be dominant in the diode saturation current. The space-charge layer recombination current density J_{0r} is given by

$$J_{0r} = qn_i WD/2L^2, \quad (20)$$

where the diffusion length L and diffusion coefficient D in the n-GaAs layer are used for those in the space-charge region. This is because most of the space-charge region is in the n-GaAs. In Eq. (20), q is the electronic charge, n_i is the intrinsic carrier concentration and W is the space-charge layer width. The dislocation density dependence of thin-film AlGaAs-GaAs heteroface solar-cell properties were calculated using the usual theoretical equation for solar-cell property[12] and Eqs. (12)–(20).

In the calculation, reflection loss due to a Si_3N_4 antireflection (AR) coating on top of the AlGaAs layer was included according to the reported data.[13] Furthermore, a realistic series resistance was considered and the series resistance R_s of the cell was calculated using a method prescribed by Handy.[14] A typical value of R_s, which depends on the junction depth, is taken to be 0.5 Ω for a nine grid line 1×1 cm^2 cell having a junction depth of 0.5 μm.

In the thin-film GaAs heteroface solar cells, recombination loss at the interface between GaAs and Si is also dominant because of a large lattice mismatch of about 4%. Figure 5 shows changes in interface recombination velocity S_I for the InGaP/GaAs system[15] as a function of lattice mismatch $\Delta a/a_0$. In the GaAs/Si system, loss due to the interface recombination velocity is expected to be about 5×10^6 cm/s from $\Delta a/a_0$ of 4×10^{-2} and was included in the calculation.

The heteroface solar-cell properties were calculated assuming zero-contact shadowing loss under AM0 illumination and 300-K temperature. The physical parameters used in the calculations are listed in Table I.

IV. EFFICIENCY CALCULATION OF GaAs HETEROFACE SOLAR CELL

Figure 6 shows calculated cell efficiency and short-circuit current density for AlGaAs-GaAs heteroface thin-film solar cells as a function of the dislocation density. The physical parameters listed in Table I are used in the calculation. In this figure, the experimental data for AlGaAs-GaAs heteroface solar cells on Si of Matsuda[16] and the corrected values for the homojunction GaAs cells on Si of Fan *et al.*[4] have been compared with those of the AlGaAs-GaAs heteroface solar cells on GaAs[17] and Ge substrates.[18] The good agreement between experimental and theoretical values indicates the validity of the model calculation. At this stage, the low efficiency of the thin-film GaAs solar cells on Si substrates is attributed to recombination loss at dislocations whose density is about 10^7 cm^{-2} in those cells. The results

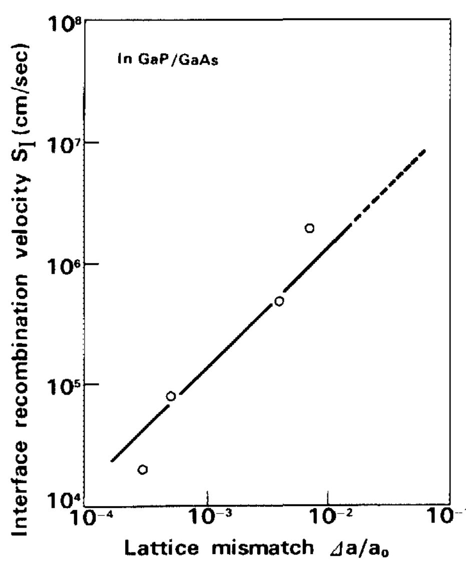

FIG. 5. Changes in interface recombination velocity S_I as a function of lattice mismatch $\Delta a/a_0$ for InGaP/GaAs heteroepitaxial interface.[15]

TABLE I. Physical parameters for AlGaAs-GaAs heteroface cell.

Layer	Parameter	Symbol	Value
p^+-AlGaAs window layer	AlAs content	x	0.85
	Layer thickness	x_1	$0.1\ \mu m$
	Carrier concentration	p_1	$5\times10^{18}\ cm^{-3}$
	Electron diffusion length	L_{n1}	$L_{n2}/2$
	Surface recombination velocity	S	5×10^{6} cm/s
p-GaAs layer	Carrier concentration	p_2	$5\times10^{18}\ cm^{-3}$
	Electron diffusion length	L_{n2}	Eq. (17)
	Electron diffusion constant	D_{n2}	Eq. (12)
	Junction depth	x_j	$0.5\ \mu m$
n-GaAs	Carrier concentration	n	$1\times10^{17}\ cm^{-3}$
	Hole diffusion length	L_p	Eq. (18)
	Hole diffusion constant	D_p	Eq. (13)
	Layer thickness	x_n	$4.5\ \mu m$

indicate a need for dislocation density lower than $10^6\ cm^{-2}$ for solar cells having a practical efficiency of 18% (intrinsic efficiency of 20%) or more. Further reductions in dislocation density are required in the fabrication of high-quality GaAs layers on Si substrates to realize high efficiency thin-film GaAs solar cells. It is particularly necessary to improve the interfacial layers such as thin Ge,[3,4] low-temperature deposited GaAs,[19] and superlattice[20] layers. These layers act as crystal nuclei of GaAs and as barriers to propagation of dislocations from the interface between the interfacial layer and Si.

Figure 7 shows calculated solar-cell parameters for the AlGaAs-GaAs heteroface thin-film solar cells as a function of the dislocation density. Since a decrease in the minority-carrier diffusion length and an increase in the recombination

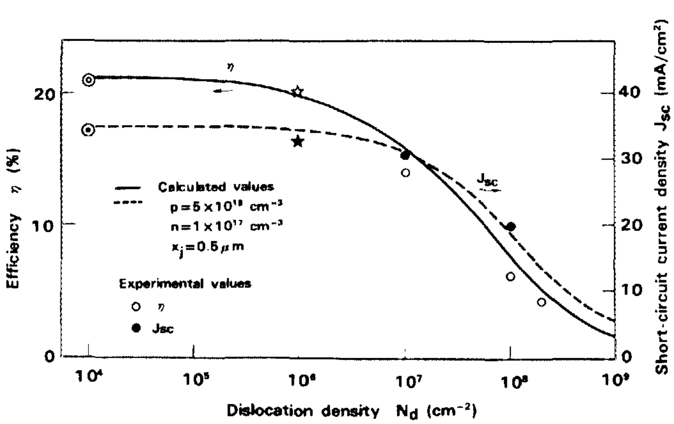

FIG. 6. Calculated AM0 conversion efficiency and short-circuit current density for p^+-p-n AlGaAs-GaAs heteroface thin-film solar cells on Si substrates as a function of dislocation density, in comparison with the experimental values for heteroface AlGaAs-GaAs solar cells on Si of Matsuda[16] and homojunction GaAs cells on Si of Fan *et al.*[4] The double circles and star-shaped symbols show the experimental data for p^+-p-n AlGaAs-GaAs heteroface solar cells on GaAs[17] and those on Ge[18] substrates.

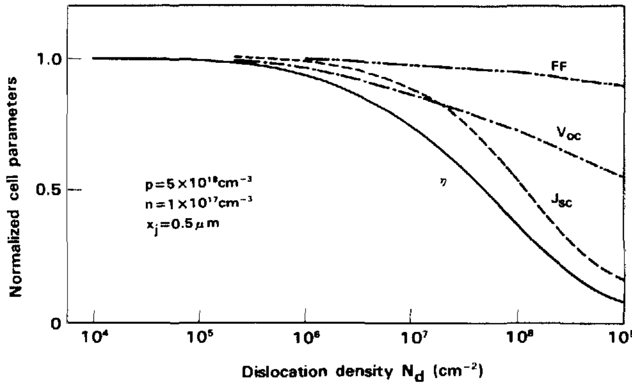

FIG. 7. Calculated solar cell parameters under AM0 illumination for p^+-p-n AlGaAs-GaAs heteroface thin-film solar cells as a function of dislocation density in the GaAs thin-film layer.

current density results from increases in the dislocation density of a GaAs thin-film layer, short-circuit current density, and open-circuit voltage mainly decrease with the increase in dislocation density.

V. NUMERICAL ANALYSIS OF HETEROFACE THIN-FILM CELL STRUCTURE

In this section, the numerical analysis results for optimization of thin-film AlGaAs-GaAs heteroface solar-cell structure will be analyzed. The n^+-n-p heteroface cell will also be analyzed as well as the p^+-p-n heteroface cell shown in Fig. 1. In these calculations, the aluminum context x in the $Al_xGa_{1-x}As$ window layer was taken to be 0.85 and the window layer thickness x_1 was taken to be $0.1\ \mu m$.

Figure 8 shows calculated AM0 conversion efficiency versus p-GaAs layer carrier concentration for the thin-film p^+-p-n heteroface solar cells with a junction depth of $0.5\ \mu m$ and n-GaAs layer carrier concentration of $1\times10^{17}\ cm^{-3}$ as a function of dislocation density. Although strong p-GaAs layer carrier concentration dependence on cell efficiency

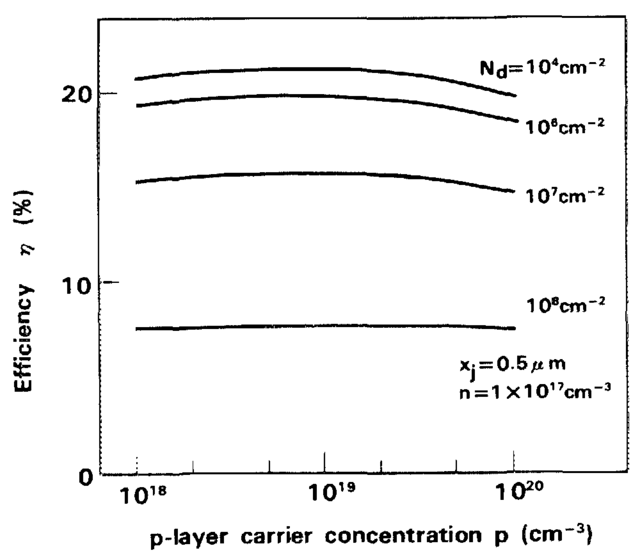

FIG. 8. Calculated AM0 conversion efficiency vs p-GaAs layer carrier concentration for thin-film p^+-p-n AlGaAs-GaAs heteroface solar cells with a junction depth of $0.5\ \mu m$ and a n-GaAs layer carrier concentration of $1\times10^{17}\ cm^{-3}$ as a function of dislocation density.

was not observed, an increase in p-GaAs layer carrier concentration tends to cause an increase in the build-up voltage, and decreases in short-circuit current density and series resistance. Thus, in the following calculations, the p-GaAs layer carrier concentration for thin-film GaAs cells was taken to be 5×10^{18} cm^{-3}.

Figure 9 shows calculated AM0 conversion efficiency versus junction depth for the thin-film p^+-p-n and n^+-n-p heteroface solar cells as a function of dislocation density. For a p^+-p-n heteroface solar cell with lower dislocation density, a junction depth x_j of 0.5–0.7 μm is optimum for a high-efficiency cell. This is because collecting photogenerated carriers with large diffusion length in the p-GaAs layer results in high efficiency. Optimum junction depth for a high efficiency p^+-p-n heteroface cell becomes shallower as dislocation density increases, because of the decrease in diffusion length in the p-GaAs layer due to the increase in dislocation density. In a solar cell with a shallow junction of less than 0.2 μm, the n^+-n-p heteroface cell structure was found to be more highly efficient than the p^+-p-n cell. In the n^+-n-p heteroface solar cells, a shallow junction cell which can collect photogenerated carriers with large diffusion length in the p-GaAs was found to be useful for a high-efficiency solar cell.

Figure 10 shows calculated AM0 conversion efficiency versus n-GaAs layer carrier concentrations for thin-film p^+-p-n heteroface solar cells, with a p-GaAs layer carrier concentration of 5×10^{18} cm^{-3} and a junction depth of 0.5 μm as a function of dislocation density. Although the n-GaAs layer carrier concentration dependence on cell efficiency is not clear, an increase in n-GaAs layer carrier concentration tends to cause an increase in built-in voltage and a decrease in short-circuit current density. Thus, the optimum n-GaAs layer carrier concentration for high efficiency thin-film p^+-p-n GaAs heteroface solar cells was found to be about 1×10^{17} cm^{-3}.

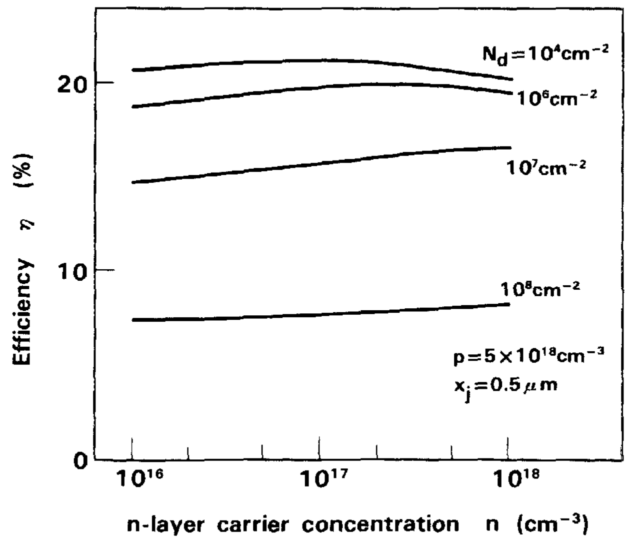

FIG. 10. Calculated AM0 conversion efficiency vs n-GaAs layer carrier concentrations for thin-film p^+-p-n heteroface solar cells with a p-GaAs layer carrier concentration of 5×10^{18} cm^{-3} and a junction depth of 0.5 μm as a function of dislocation density.

Figure 11 shows the calculated AM0 conversion efficiency for the p^+-p-n and p^+-p-n-n^+ structure heteroface GaAs thin-film cells with a p-GaAs layer carrier concentration of 5×10^{18} cm^{-3}, a junction depth of 0.5 μm and an n-GaAs layer carrier concentration of 1×10^{17} cm^{-3} as a function of n-GaAs layer thickness. The p^+-p-n-n^+ structure is more useful for high efficiency cells compared to the p^+-p-n cell structure. This is because the n^+ layer provides a back-surface field, minimizing recombination losses at the interface with the Si substrates. For GaAs, a 2-μm-thick n layer was found to be able to generate over 95% of the maximum photogenerated photocurrent produced by an infinite thickness. Therefore, it is estimated that thin-film GaAs heteroface solar cells, when fully developed, will achieved practical

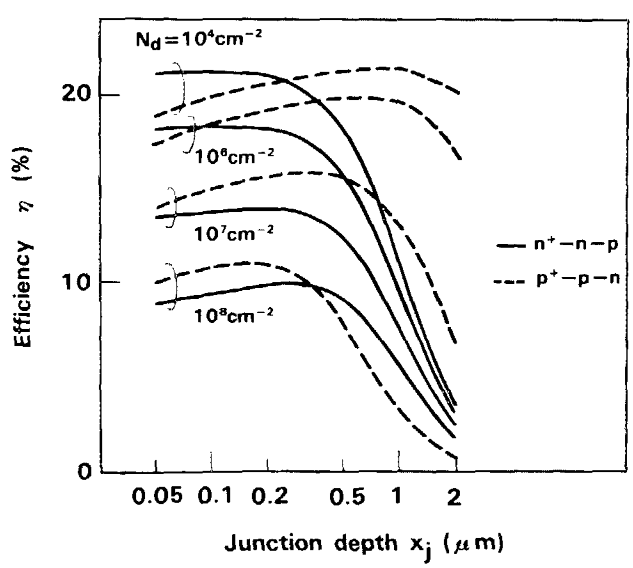

FIG. 9. Calculated AM0 conversion efficiency vs junction depth for thin-film p^+-p-n and n^+-n-p heteroface solar cells with upper p- and n-layer carrier concentrations of 5×10^{18} cm^{-3} and bottom n- and p-layer carrier concentrations of 1×10^{17} cm^{-3} as a function of dislocation density.

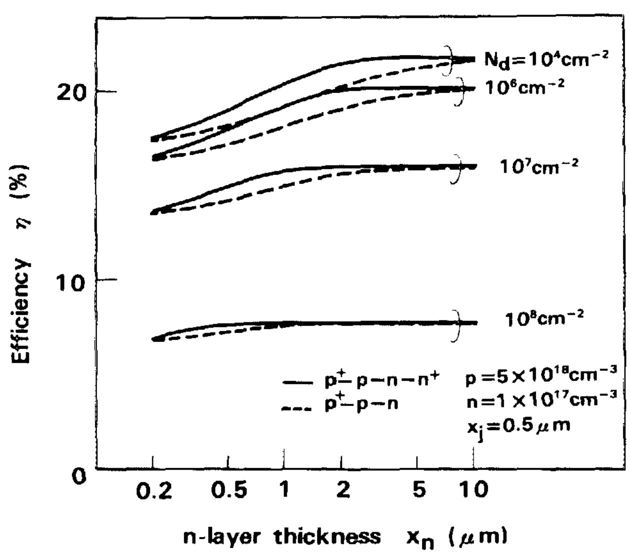

FIG. 11. Calculated AM0 conversion efficiency for p^+-p-n and p^+-p-n-n^+ structure heteroface AlGaAs-GaAs thin-film solar cells with a p-GaAs layer carrier concentration of 5×10^{18} cm^{-3}, a junction depth of 0.5 μm and an n-layer carrier concentration of 1×10^{17} cm^{-3} as functions of n-GaAs layer thickness and dislocation density.

efficiencies as high as 18% (intrinsic efficiency of 20%) with GaAs layers only 3 μm thick.

VI. SUMMARY

The effects of dislocation on the efficiency of single-crystal thin-film AlGaAs-GaAs heteroface solar cells on Si substrates has been analyzed. Solar-cell properties were calculated based on a simple model in which dislocations act as recombination centers, reduce minority-carrier diffusion length in each layer, and increase the space-charge layer recombination current. Excellent agreement between the theory and experiments indicates that recombination loss at dislocations is the predominant loss mechanism in thin-film AlGaAs-GaAs heteroface solar cells and one could fabricate thin-film cells with a practical efficiency larger than 18% on Si substrates if the dislocation density in the thin-film GaAs layer is less than 10^6 cm^{-2}.

Numerical analysis was also carried out to optimize the thin-film AlGaAs-GaAs heteroface solar-cell structures. Computer calculations show that an n^+-n-p heteroface cell structure is more efficient in a solar cell with a shallow junction less than 0.2 μm, while a p^+-p-n heteroface cell structure is more efficient in a deep junction solar cell. In the p^+-p-n heteroface solar-cell structure, optimum values of p-GaAs layer carrier concentration, junction depth, n-GaAs layer carrier concentration and n-GaAs layer thickness, for high efficiency solar cells,were found to be 5×10^{18} cm^{-3}, 0.5 μm, 1×10^{17} cm^{-3}, and 2–5 μm, respectively.

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