

**Studies of High Efficiency $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{Si}$ Tandem
Solar Cells Grown by MOCVD**



Contents

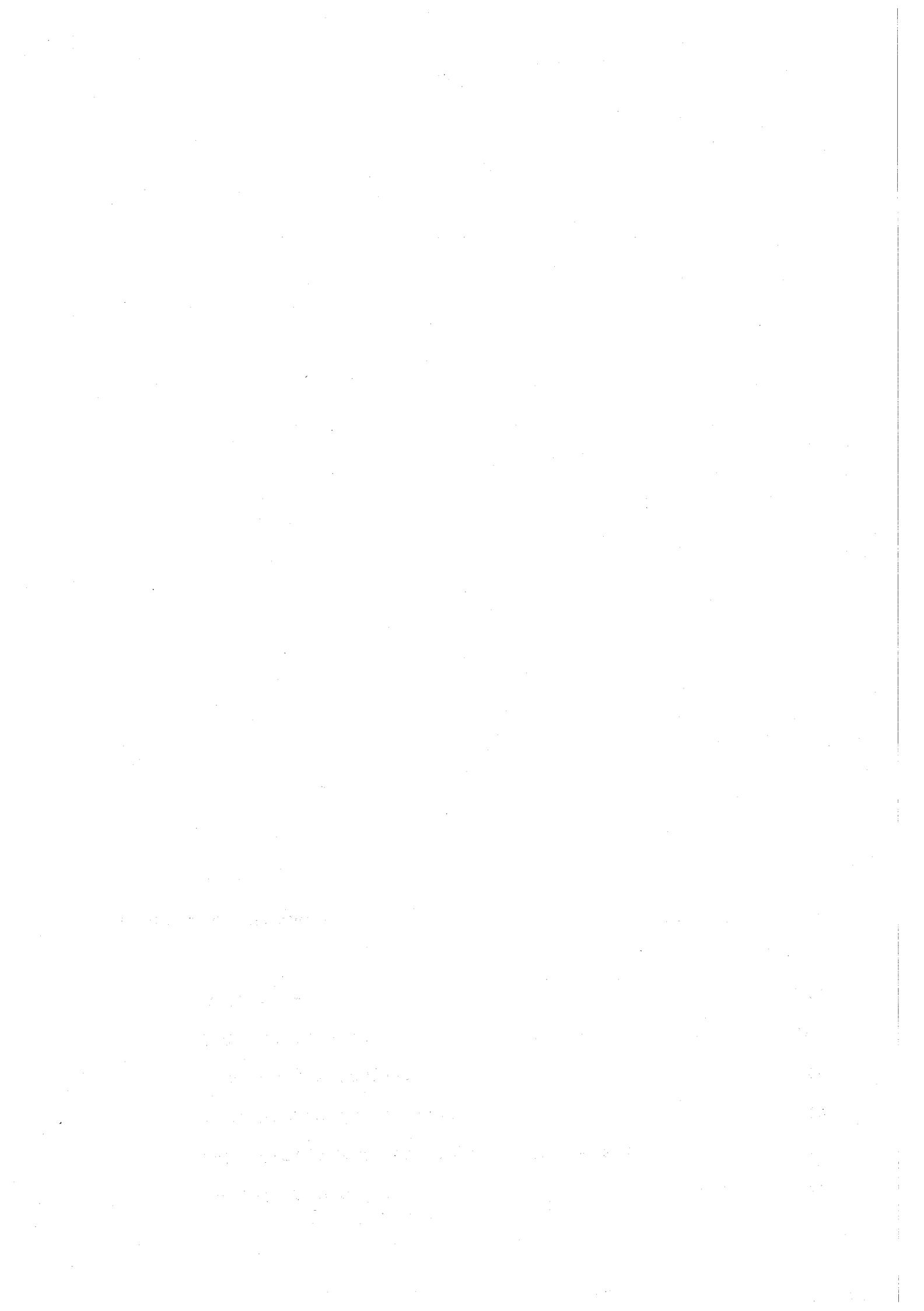
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Chapter 1. Introduction

1-1. Background

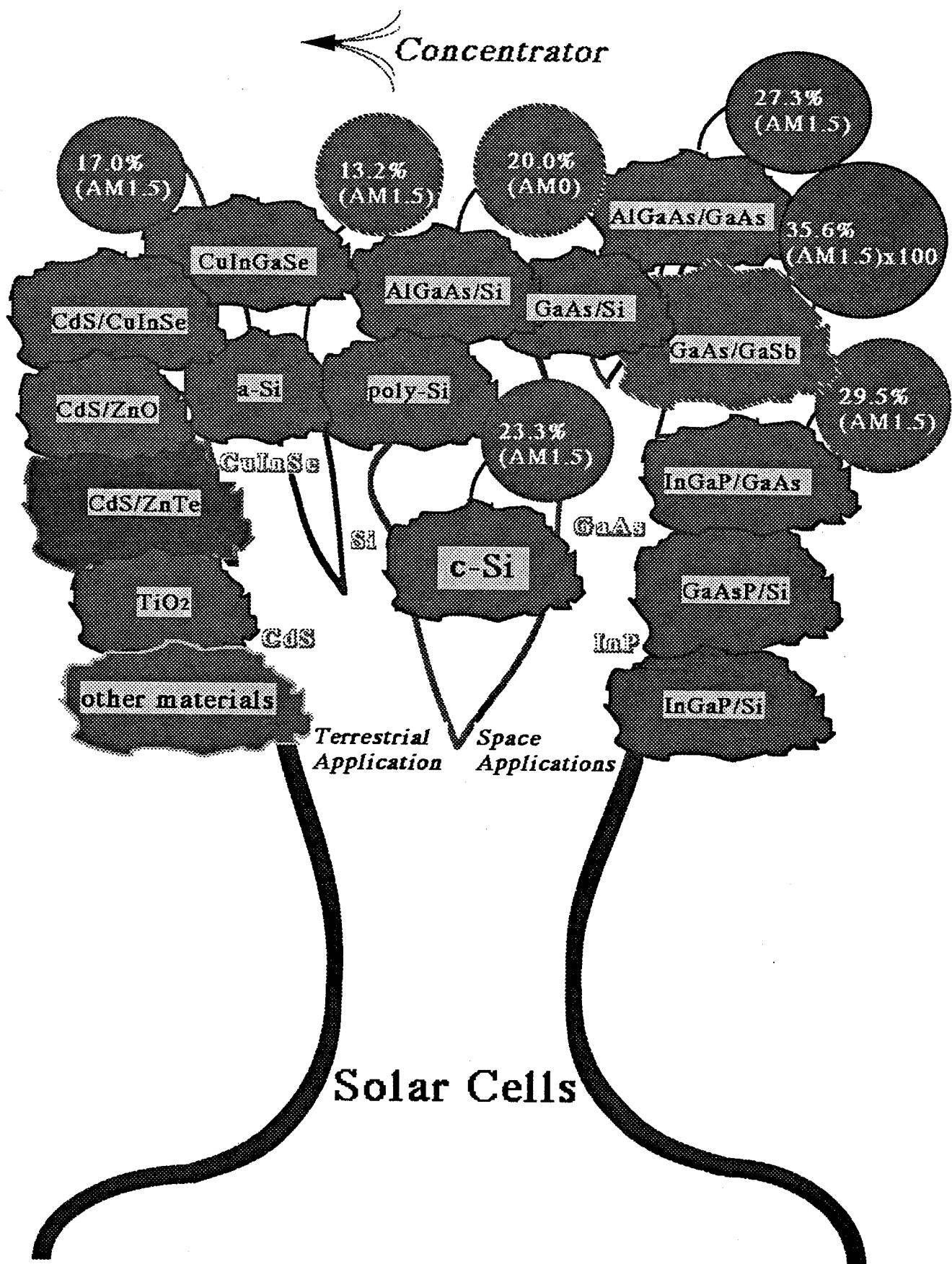
The photovoltaic effect was discovered by E. Becquerel in 1839 in an electrolytic solution. About 40 years later the effect was noted in a selenium structure and next much research was done on the cuprous oxide devices, but the conversion efficiency was never achieved beyond 0.5%. It was used in camera exposure meters and photoelectric sensors. In the later 1940's, a p-n junction germanium photocell with extremely small area was developed as a detector rather than a power source. When single crystalline silicon became available, p-n junctions were made by a variety of techniques, e.g., alloying an impurity such as aluminum, beta particles bombardment, thermal diffusion method, and so on. In 1953, a Si photovoltaic cell showed greater than 1% conversion efficiency. Since that time, many successful techniques were developed rapidly. The field of photovoltaic energy conversion is entered into the modern era ¹⁾. By mid-1957, the efficiency of Si solar cell was increased to 8%, and it was the first time that Si solar cells were applied in space powering the electronic devices and their experiments for the Vanguard satellite of America on March 17, 1958.

Until 1959, the efficiency of solar cell was up to 14% level. After that time, many semiconductor materials have been developed for solar cells, such as poly-Si, a-Si, CdS, CuInSe, GaAs and so on. It is clear that the exploration of space would not have been so rapid or successful without solar

cells. However, it is most significant to today that solar cells are used competitively to generate power on the earth's surface as a stable clear energy source. This is an important technology to meet the world's demands in the future for a gap between energy required for humankind and production volume of fossil fuels in the emergence of severe global environmental problems. A lot of researches and developments were aimed at the practical realization of terrestrial photovoltaic power generation. In the past 10 years, there has been a great progress in reducing the cost, increasing the efficiency and increasing the lifetime of photovoltaic cells and modules. The conversion efficiency for small-area solar cell in laboratory varies from 18% to 23% for c-Si base cells, 12 to 18% for poly-Si cells, 5% to 13% for a-Si base cells, 20% to 29% for GaAs base cells and 11% to 16% for CuInSe base cells. The developments of solar cells are described briefly in Fig. 1-1.

Further improvements in conversion efficiency and reduction of costs are anticipated from use of the device design of novel structure, processing and measurement of material, forward understanding in device physics, materials and cell properties.

Monolithic tandem solar cell has attracted attention as the most interesting approach in order to achieve a high efficiency over 30%. Some tandem solar cells have been investigated for more than decade in the search for a material system of high-efficiency. On the point of economic reason, and considering the advantage of Si in abundance of material,



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Fig.1-1 Developments of the modern solar cells

high technology developed and in large-area, strong mechanical strength, we preferred Si as a bottom cell material. The GaAs-AlGaAs system is a very attractive candidate for the top cell material. Despite some difficulties to be overcome, it is very significant to develop the tandem solar cell for achieving a high-efficiency, low cost and large-area tandem solar cell.

Solar cells can surely be considered a key technology for overcoming global environmental problems and energy problems. It can be seen that the most important factors for solar cell application are high efficiency and low cost. We hope the photovoltaic era is coming in the future with R & D progress in solar cells.

1-2. Heteroepitaxial growth of GaAs on Si

GaAs was first grown on Si substrate using Ge as the intermediate layer ²⁾, as the lattice constant and the thermal expansion coefficient of Ge approximates to that of GaAs. GaAs can be relatively easily grown on Ge substrate ³⁻⁷⁾. After Ge was formed on Si substrate by a vacuum evaporation, GaAs was grown on it ⁸⁻¹⁰⁾. But the crystallinity of GaAs is greatly affected by the surface condition of Ge on Si, and the GaAs heteroepitaxial layer is contaminated by Ge due to its high vapor pressure. Although some devices have been grown on the Ge/Si substrate, such as, solar cell ¹¹⁻¹³⁾, FET's ^{14, 15)}, LED's ^{16,} ¹⁷⁾, laser ^{18, 19)}, characteristics of these devices are unsatisfactory with Ge as an intermediate layer.

Since the first report of successful heteroepitaxial growth of GaAs on Si directly in 1984 ^{20, 21)}, the epitaxial growth technology of GaAs on Si has been developed actively. The crystal quality has been continuously improved. The most popular technique to grow GaAs on Si substrate is two-step growth method ²²⁻²⁴⁾, however, GaAs growth on Si involves following problems:

- 1) High density of misfit dislocations due to about 4.1% difference in the lattice constants.
- 2) Residual stress caused by the difference in the thermal expansion coefficients between Si and GaAs. At the room temperature, the thermal expansion coefficient of GaAs is about 2.5 times larger than that of Si.
- 3) The generation of anti-phase domain takes place as polar

semiconductor is grown on a nonpolar semiconductor²⁵⁻²⁸⁾.

4) There is relatively low resistivity of undoped layer due to unintentional Si auto-doping²⁹⁻³²⁾. The carrier concentration in the undoped GaAs layer on GaAs is about 10^{14} cm⁻³ range using the metal-organic chemical vapor deposition (MOCVD) technique, but undoped GaAs layer on Si have the concentration in the $10^{16} \sim 10^{17}$ cm⁻³ with n-type conductivity.

5) There is a relatively rough surface morphology in comparison with that grown on GaAs substrate³³⁻³⁶⁾.

Many technique for crystallinity improvement of GaAs on Si have been attempted, e.g., use of a strained layer superlattice (SLS)³⁷⁻⁴¹⁾, in-situ and ex-situ thermal cycle annealing (TCA)⁴²⁻⁴⁴⁾ and a combination of these techniques^{45, 46)}. The crystalline quality has been continuously improved. However, the most suitable technique to reduce the dislocation density to below 1×10^4 cm⁻² has not yet been found.

1-3. Device application

In recent years, the heteroepitaxial growth of GaAs on Si has received great attentions because of numerous potential applications for monolithic integration of GaAs and Si optoelectronic devices and circuits ⁴⁷⁻⁵⁹⁾. More substantial benefits of monolithic GaAs/Si technology is its application to solar cells. However, the main problems which occur against device application are the generation of the high density of dislocations and the residual stress in the epitaxial layer caused by the lattice mismatch and the difference of the thermal expansion coefficient.

Some successful application of GaAs on Si to majority carrier devices have been so far reported, e.g., the metal-semiconductor⁶⁰⁾ and modulation-doped field-effect transistor⁶¹⁾. The characteristics of GaAs devices on Si are close to those of GaAs on GaAs. Because the characteristics of the majority carrier devices are not greatly affected by the dislocations, and the total epitaxial layer is relatively thin for these devices, cracks are not generated. But the unintentional Si autodoping still affects pinch-off characteristics of metal-semiconductor effect transistors and high electron mobility transistors (HEMT's) on Si .

On the other hand, the characteristics of minority carrier devices are seriously affected by the dislocations ^{30,}
⁶²⁾ and stress. The cw threshold current of AlGaAs/GaAs laser on Si increased by a factor of 3 in 10 hours ⁶³⁾, and appeared in short device lifetime at room-temperature cw operation

⁶⁴⁻⁶⁶⁾. The reason of these rapid degradation is the formation and propagation of dark-line defects, because the active layer of AlGaAs/Si laser on Si is not only subject to high tensile stress but also contains a high density of threading dislocations. The dislocations acting as nonradiative recombination centers which degrade the crystallinity of heteroepitaxial layer resulting in short minority carrier lifetimes. The short minority carrier lifetime makes the conversion efficiency of solar cell low. C. C. Fan et al. have reported the GaAs/Ge/Si with the efficiency of 14.1% (AM1.5), which solar cell uses Ge layer as an intermediate layer between the GaAs film and the Si substrate ⁶⁷⁾. The high efficiency of 18.3% (AM0) and 20%(AM1.5) for GaAs solar cell have been achieved by Yamaguchi et al. ⁶⁸⁾. M. Umeno et al. reported the AlGaAs/Si tandem solar cell with the efficiency of 20.6% (AM0) ⁶⁹⁾. The status of solar cells in the efficiency today is tabulated in Table 1-1.

Table 1-1 Status of solar cells in the efficiency today

Cell	Structure	η (%)	Affiliation	Ref.
<u>Si</u>				
c-Si	PERL	23.1 (AM1.5)	UNSW	[70]
Poly-Si	PESC	17.8 (AM1.5)	UNSW	[71]
a-Si	a-Si/a-C	13.2 (AM1.5)	Mitsui Toatsu	[72]
<u>II-VI Semiconductors</u>				
CdTe	CdTe/CdS	15.8 (AM1.5)	SFU	[73]
<u>I-III-VI Semiconductors</u>				
CuInSe ₂	ZnO/Cu(InGa)Se	15.9 (AM1.5)	NREL	[74]
<u>III-V Semiconductors</u>				
Single-Junction				
GaAs	GaInP WL	25.7 (AM1.5)	NREL	[75]
	AlGaAs WL	21.8 (AM0)	Spire	[76]
	GaAs on Si	18.3 (AM0)	NTT	[77]
	GaAs on Ge	20.1 (AM0)	ASEC	[78]
InP	Graded-junction	19.1 (AM0)	Spire	[79]
Two-Junction				
InGaP/GaAs	AlInP ₂ WL	29.5 (AM1.5)	SERI	[80]
AlGaAs/GaAs	Metal-interconnect	23.0 (AM0)	Varian	[81]
GaAs/GaSb	MSMJ	30.5 (AM0) × 50	Boeing	[82]
GaAs/Si	Tunnel-interconnect	19.5 (AM0)	NIT	[83]
AlGaAs/Si	Tunnel-interconnect	20.6 (AM0)	NIT	[69]
Three-Junction				
AlGaAs/GaAs/InGaAs	Tunnel-interconnect	25.2 (AM0)	Varian	[84]

1-4. The purpose and organization of this dissertation

There are numerous potential applications to be attractive with GaAs/Si growth technology although there still remain some obstacles to be overcome in the crystallinity of GaAs/Si. The most significant application of GaAs/Si is in solar cell. GaAs/Si solar cells with tandem configuration are promising in the achievement of high efficiency and low cost solar cells. In order to transform the GaAs/Si into useful technology, studies of the material and the device characteristics of GaAs/Si are necessary and important.

This dissertation is composed of five chapters. The summary is as follows.

Chapter 1 is an introduction of this dissertation reviewing the historical development, and describes the development of heteroepitaxial growth of GaAs on Si and its applications to devices. The important results of solar cells obtained by experiments up to the present are also summarized in a table.

In Chapter 2, the material properties and the parameters of GaAs, AlGaAs, Si and GaAs-on-Si were described in general. The theoretical calculation and design for high efficiency $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{Si}$ tandem solar cells were carried out. The structure design and the parameters optimization are concentrated on GaAs/Si tandem solar cells in three-terminal configuration and on AlGaAs/Si tandem solar cell in two-terminal configuration, respectively. The photovoltaic properties of $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{Si}$ tandem solar cells were analyzed and described by the

3-dimensional graphics. The calculated results are shown.

In Chapter 3, GaAs/Si three-terminal monolithic tandem solar cells fabricated by MOCVD were studied. The "As auto-doping effect" and the effects of the GaAs growth on the Si bottom cells were investigated by the SIMS and EBIC. The main reasons for the achievement of the high efficiency tandem solar cell are described in detail. It is that the performances of the GaAs top cell was considerably improved by using a graded-bandgap-layer of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and the high temperature thermal cycle annealing and the quantum efficiency of the Si bottom cell in the long wavelength is enhanced by using p-Si substrate with proper resistivity ($10 \Omega\cdot\text{cm}$) and BSF structure. As a result, the total conversion efficiency (active-area efficiency) of 19.9% under 1 sun, AM0 measurement conditions has been achieved by the GaAs/Si three-terminal monolithic tandem solar cell.

In Chapter 4, the characteristics of the $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{Si}$ two-terminal tandem solar cells were studied. The quantum efficiency of the Si bottom cell was improved clearly by the BSF structure in the long-wavelength region, and the conversion efficiency of the Si bottom cell is increased. Using a growth sequence with a high growth temperature (800°C) and thermal cycle annealing process of high temperature ($300\sim 900^\circ\text{C}$), the dislocation density of the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ top cells was decreased. The active-area efficiencies (1sun, AM0) of 19.0% and 20.0% for $\text{Al}_{0.15}\text{Ga}_{0.85}\text{As}/\text{Si}$ tandem solar cells have been obtained with two-terminal and four-terminal configuration,

respectively. The characteristics of the connector between the top cell and the bottom cell are also analyzed. The n-GaAs/p-Si heterojunction has tunnel junction properties in the experiment.

In Chapter 5, a new integrated wavelength-division photo-sensor using GaAs/Si was studied. It can be conveniently used to measure the wavelength of monochromatic light without using any filter or dispersive elements. Normalized difference of the photocurrents of this sensor is linearly dependent on the wavelength of the incident monochromatic light from 600 nm to 880 nm. Signal processing circuits can be also integrated on the same Si wafer.

Chapter 6 is the summary of this dissertation, and a scope for future work is also given.

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