MOLECULAR-BEAM EPITAXY OF GaAs/Si(001) STRUCTURES FOR HIGH-PERFORMANCE TANDEM $A^{III}B^{V}$/Si-SOLAR ENERGY CONVERTERS ON AN ACTIVE SILICON SUBSTRATE

M. A. Putyato, B. R. Semyagin, E. A. Emel’yanov, N. A. Pakhanov, and V. V. Preobrazhenskii

In the present study, a method of low-temperature atomic layer epitaxy of GaAs at the initial stage of formation of a GaAs/Si heterojunction is used for growing GaAs films with a low density of threading defects. It was shown that growth of GaAs films can take place bypassing the stage of formation of islands, provided the first monolayer of GaAs is formed by atomic layer epitaxy at low temperature (200–350 °C). A regime was found for growing the GaAs/Si films with a density of threading dislocations less than $10^6$ cm$^{-2}$, which corresponds to the best world achievements. In this mode, the GaAs/Si and $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}/\text{Si}$ structures were grown for solar-energy converters, the devices were produced, and their characteristics were measured. It is shown that during the growth of the GaAs/Si heterojunction, a p–n-junction is formed in the near-surface layer of silicon. This allows one to produce high-performance cascade converters of solar energy based on the $A^{III}B^{V}$ compounds on the active Si substrate in a single growth cycle.

Keywords: atomic-force microscopy, heterojunction, solar energy, converter.

INTRODUCTION

At present high-performance solar cells (SC) are complex multilayered structures with an expensive and massive germanium $p$–$n$-junction used as the first stage. Therefore, the development of high-performance cascade solar cells based on the $A^{III}B^{V}$ semiconductor compounds using inexpensive and durable Si substrates (i.e., replacement of the Ge $p$–$n$-junction by a silicon one) is one of the major problems of modern photovoltaics. The main problem here is high (~4%) lattice mismatch and even higher (up to 50%) mismatch of linear thermal-expansion coefficients between silicon and $A^{III}B^{V}$ compounds; the following cascades of solar cells are grown on. This circumstance does not allow one to obtain high-quality layers of semiconductor $A^{III}B^{V}$ compounds on Si (with long lifetime and high mobility of minority charge carriers), which is a necessary condition for efficient operation of solar cells.

To date, there are two ways to solve the problem of producing solar cells on active silicon substrates. The first way is to develop methods for obtaining new materials with the desired band gaps $E_g$ and lattice-matched with Si. Intensive studies in this direction related mainly with the use of nitrogen-containing $A^{III}–N–B^{V}$ compounds are under way worldwide [1]. A quaternary GaN$_x$(P$_x$As$_{1-x}$)$_{1-y}$ solid solution is considered to be most suitable for these purposes. Depending on the ratio between the components, the band gap of this material may vary from 1.5 to 2.0 eV with full lattice matching with the Si-substrate. In so doing, GaN$_x$(P$_x$As$_{1-x}$)$_{1-y}$ is a quasidirect-gap semiconductor with the absorption spectrum suitable for solar cells. However, the electrophysical parameters of such materials, above all the diffusion length of minority carriers, remain very low to date [1]. Moreover, according to the leading experts, the question on possibility of improvement of these parameters is still open [1]. The latter circumstance casts some doubt on the very prospects of this direction in principle.

Institute of Semiconductor Physics of the Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia, e-mail: puma@isp.nsc.ru; ppv@isp.nsc.ru. Translated from Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika, No. 9, pp. 26–33, September, 2010. Original article submitted June 24, 2010.
The second way is the formation of a buffer Si$_{1-x}$Ge$_x$ layer on silicon with the transition to the lattice constant of Ge, which is very close to the lattice constant of gallium arsenide. This, in principle, allows one to grow fairly high-quality $A^{III}B^V$ layers with large values of diffusion lengths of minority carriers on single crystal silicon substrates and, consequently, to obtain high-performance solar cells.

Work in this direction is also being under way fairly widely [2]. First (and good!) single-stage solar cells based on GaAs/Si$_{1-x}$Ge$_x$/Si heterostructures have already been produced using such buffer layers [3].

Note, however, that this approach has a fundamental disadvantage. It is that the buffer Si$_{1-x}$Ge$_x$ layer, whose thickness is not less than 10 $\mu$m, is opaque in the spectral region of effective photoconversion in silicon. Therefore, Si, which can be used as a very effective element of a multicycle solar cell, acts merely as an inert substrate in this case.

In cascade solar cells, it is highly desirable to use Si as an active layer. This requires a buffer layer matching the lattice constants of the substrate and the solar cell structure. This buffer must be transparent in the spectral range of Si photosensitivity.

We have chosen a third way, namely, the way related with the use of buffer layers on the basis of wide-gap $A^{III}B^V$ compounds and solid solutions Al$_{1-y}$Ga$_y$As, In$_{1-y}$Ga$_y$P, GaP$_{1-y}$As$_y$. With the corresponding composition, these materials are transparent in the spectral range of silicon sensitivity and allow the transition to the lattice constant of GaAs. This, in turn, will enable one to use them for growing compounds Al$_{1-y}$Ga$_y$As, In$_{1-y}$Ga$_y$P$_{1-y}$As$_y$, and In$(AlGa)_{1-y}$P lattice-matched with GaAs and well developed now for highly efficient solar cells. These solid solutions have the GaAs lattice constant and $E_g$ close to optimal ones. Combination of the above materials with active Si will enable one to build one of the most effective architectures of two-and three-cycle solar cells, real development of which we can discuss at the present time.

Thus, the expected efficiency for a two-cycle AlGaAs/Si or InGaP/Si solar cell with $E_g = 1.7/1.1–1.8/1.1$ eV is 44%. For a three-cycle InGaP/GaAs/Si solar cell with $E_g = 1.81/1.4/1.1$ eV, the expected efficiency is up to 47%. Note that for solar cells obtained to time on the expensive and heavy Ge or GaAs substrates, the expected efficiencies (i.e., efficiencies, which are expected to be actually achieved) are: up to 38% for a two-cycle InGaP / GaAs and up to 44% for a three-cycle InGaP/GaAs/Ge [1].

Thus, the efficiency of the cascade solar cells on the active silicon substrate is potentially even higher than that of the germanium solar cells for the same number of cascades.

A key and the most challenging issue in the production of such highly efficient cascade solar cells on active silicon is the development of a technology for obtaining a transparent buffer layer with the dislocation density less than $10^6$ cm$^{-2}$ on the basis of solid solutions Al$_{1-y}$Ga$_y$As, In$_{1-y}$Ga$_y$P, Al$_{1-y}$In$_y$P, or GaP$_{1-y}$As$_y$ by MBE [4]. In so doing, these layers should have smooth surfaces and a thickness of about 1 $\mu$m.

The direct experiments (for GaAs/Si and GaP/Si heterostructures ([5])) showed that the density of threading dislocations directly at the growth temperature can be reduced down to $10^4–10^5$ cm$^{-2}$. However, upon cooling to room temperature, it increases up to $10^5–10^7$ cm$^{-2}$. Thus, for any $A^{III}B^V$ heterosystems on the Si substrate, of critical importance is the large difference in the linear thermal expansion coefficients (LTEC) of the matched materials rather than the lattice mismatch (for example, in the GaP/Si system, it is several tenths of a percent).

This implies that lowering the growth temperature is one of the main ways of obtaining heterolayers with low density of threading dislocations. In this regard, the most suitable epitaxial technology is the method of molecular beam epitaxy (MBE) allowing gallium arsenide to be grown at 150–200°C [6].

In the present study, the technology for MBE growing relaxed, smooth, and low-dislocation (<$10^6$ cm$^{-2}$) buffer GaAs and Al$_{1-y}$Ga$_y$As layers on a silicon substrate and the development of heterostructures based on these layers for high-efficiency multicycle solar energy converters on the active silicon substrate were discussed.

**EXPERIMENTAL**

The heterostructures under study were grown using a modernized “Shtat” MBE facility. In the experiment, used was made of the Si (001) substrates declined by $6^\circ$ in the [110] direction. To obtain the Ga, Al, and In fluxes, solid-state molecular sources (MS) were emplyed. The fluxes of As$_2$ and P$_2$ molecules were produced by means of valve sources with a cracking [7]. The setup was equipped with a high-energy electron reflection diffractometer. The flux density of