On modelling optical parameters of InAs quantum dots for cascade GaInP / GaAs / Ge solar cells

A N Panchak, S A Mintairov, M A Mintairov, R A Sali, M Z Shvarts and N A Kalyuzhnyy

Ioffe Institute, Polytechnicheskaya Str. 26, St. Petersburg, Russia, 194021
E-mail: a.panchak@mail.ioffe.ru

Abstract. Triple-junction solar cells InGaP/GaAs/Ge usually are manufactured using MOCVD technology. However, the potential of such structures is investigated in the laboratory on samples made using MBE. One of the ways to increase efficiency is the implanting of InAs quantum dots in GaAs cascade. In this paper the approaches to the mathematical modeling of Ga (In) As structures grown by MOCVD and MBE are studied.

1. Introduction

Triple-junction solar cells InGaP/GaAs/Ge today have one of the highest efficiency among photovoltaic (PV) cells produced for mass market. They include p-n junctions (sub-elements) with different widths of the band gap for operation in three spectral diapasons. It reduces the losses on thermalization of charge carriers and incomplete absorption of radiation. One of the features in three-junction SCs is the non-equivalent current generation in sub-elements. So, the largest photocurrent is generated in the lower Ge sub-cell. The expansion of the GaAs subcell spectral sensitivity to the long waves can increase its current generation due to the lower subcell and increase the PV conversion efficiency [1]. This is possible through the implanting of InAs quantum dots (QDs)array into GaAs subcell.

In laboratory conditions, InAs QDs in a GaAs host are produced usually, in MBE process. So, for example, structures with 30 layers of QDs were previously investigated [2]. The lateral average size of QDs was about 16 nm, and their height was about 6 nm. However, on PV mass market MBE technology is not spread out because it does not provide a cost-effective manufacturing of large-area devices.

In industry the MOCVD technology provides large area devices in one manufacturing process at higher growth rates. Earlier, for the GaAs PV cells, the MOCVD technology was developed [3,4] structural perfection of QDs grown by this method was not inferior of the MBE QDs.

The difference in production methods greatly influences the final design of the fabricated structure. It leads to a different approach to the mathematical modeling of devices produced by the MOCVD and MBE method. This paper is devoted to the study of approaches to modeling InAs QDs in the GaAs host material for PV cells.

2. Properties of MOCVD and MBE structures in terms of mathematical modelling

A thin wetting layer is first formed in the growth process of InAs QDs in the host GaAs material. QDs themselves are formed lather on the Stranski-Krastanov mechanism. The production of QDs is non-uniform over the entire area of the device; therefore, there is a variation in the size of quantum dots.
In mathematical modeling of optical parameters of a structure with quantum objects, their size plays an important role. It determines the position of the levels of bounded states produced by the restriction of charge carriers in one dimension in the case of a thin film (quantum well) or in three dimension in the case of a quantum dot. The position of the energy levels in QD material on the one hand is limited by band offsets and on the other hand by the valence band and conduction band of host material. In the first case, the studied quantum objects cease to be quantum, since their sizes become so large that in the region limited by the main material the spectrum becomes quasi-continuous. In the second case, the quantum object is so small that there is not a single allowed energy value between the conduction band and the valence band of the host material.

MBE manufactured GaAs PV converters with InAs quantum dots array of 30 layers with $4 \times 10^{10} \text{cm}^{-2}$ dot density were studied in [2]. The results of a TEM study of this structure, as well as the distribution of QD by lateral and vertical dimensions appear in figure 1.

The dimensions of the quantum dots here are 8 nm in the vertical direction and 16 in the lateral direction. This is the only pronounced QD size. This size was taken as the basis for the mathematical modeling of the internal quantum yield of this structure. The thickness of the wetting layer, determined from TEM studies, was 0.3 nm. Comparison of the results of mathematical modeling and measurement results appear in figure 2.
Photovoltaic converters manufactured by MOCVD technology had 10 layers of InAs QDs [3]. The density of dots per layer was $7.5 \times 10^8 \text{ cm}^{-2}$. The results of a TEM study of this structure, as well as the distribution of CT in lateral and vertical dimensions appear in figure 3.

![Figure 3](image1)

**Figure 3.** Results of a TEM study (a), as well as the size distribution of QD in the vertical direction (b) and lateral direction (c) for the InAs/GaAs structure manufactured by MOCVD technology. The results given for vertical dimensions were obtained using TEM studies, the results given for lateral direction were obtained using AFM studies.

The growth parameters were selected in the MOCVD process in such a way that the InAs/GaAs QDs had dimensions similar to those of the QD obtained in MBE process. So were made PV converters with QDs of 16 nm in the lateral direction and 6 nm in the vertical direction. However a bimodal distribution of QD sizes was observed. Also QDs of 9 nm in the lateral direction and 2 nm in the vertical direction abound [4]. This character of the size distribution of QDs comes due to the process of their formation. In the case of MOCVD, on the wetting layer, first, appear QDs of small sizes, which grow and merge later. With a bimodal size distribution of QDs, mathematical modeling using a medium size will not give a satisfactory result. Therefore, the calculation should be carried out for "small" and "large" points, taking into account their quantitative distribution.

The wetting layer thickness in the sample produced by MOCVD technology was 1.2 nm. The thickening of the wetting layer leads to a decrease in absorption long wave edge. For the studied sample, this was reflected in a significant increase in the internal quantum yield in the region of 1.3 eV.

Comparison of the results of mathematical modeling and measurement results appear in figure 4.

![Figure 4](image2)

**Figure 4.** Internal quantum yield of InAs/GaAs QD PV converter manufactured by MOCVD. The numbers denote (1) the measured data and (2) the calculation results. Data are given in terms of 1 layer.
The density of quantum dots in the case of MOCVD is significantly less than in the case of MBE. For this reason, it is difficult to estimate the contribution of “large” points, since it is comparable in magnitude with the measurement error. The substantially high IQY value in the case of MOCVD is due to the wide wetting layer. Since the edge of its spectral sensitivity is located at 1.3 eV.

3. Conclusion
In this article approaches to modeling the internal quantum yield of arrays of InAs quantum dots in the GaAs base material, produced using MOCVD and MBE were studied. The growth characteristics of the structures for each method affect the size distribution of quantum dots. So in the case of MBE, this distribution is close to Gaussian. In the case of MOCVD, it is bimodal. Therefore, for mathematical modeling of the optical parameters of these structures in the case of MBE, it suffices to take the average size of QDs as the main one. In the case of MOCVD, it is necessary to carry out a calculation for the two main sizes of QDs, as well as to take into account the quantitative size distribution.

In addition, the wetting layer thickness is different in the case of MBE and in the case of MOCVD. Thus, in the case of MBE, the thickness of the wetting layer is insignificant and, therefore, slightly changes the absorption edge of GaAs. In the case of MOCVD, the wetting layer thickness is significantly greater. Therefore, it makes a significant contribution to the internal quantum yield of the structure.

References
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