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An Enhanced Charge Carrier Separation in a Heterojunction Solar Cell with a Metal Oxide

*A. L. Danilyuk, T. N. Sidorova, V. E. Borisenko, Hong Wang, Rusli Rusli, and Chenjin Lu**

A model of charge carrier transport in heterojunction solar cells composed of a solar light-absorbing semiconductor and a wide-bandgap semiconducting metal oxide is proposed. It describes an electric field in the semiconductor originating from the difference in the electron work functions between the two contacting materials, an enhanced hole separation by this field, and subsequent trap-assisted tunneling of holes through the semiconducting oxide. The model predicts a dramatic influence of the donor concentration in the semiconductor, trap parameters in the oxide, and ideality factor of the semiconductor/oxide heterojunction on the performance of the cell. The efficiency of the solar energy harvesting by MoO_x/n-Si solar cells is calculated to reach 23% of the donor concentration in Si of 10^{18} cm^{-3} at a limited hole current density. It is predicted to be reduced to 16–18% when donor concentration is in the range of 10^{15}–10^{16} cm^{-3}. The numerical predictions agree well with experimental data, at least for donor concentrations in Si below 10^{18} cm^{-3}, confirming suitability of the model for heterojunction solar cells composed of other semiconductors and semiconducting metal oxides.

1. Introduction

Metal oxides are receiving extended interest for different applications in electronics starting from thin-film transistors and memory cells to photoelectric elements and solar cells.[1–5] Some of them have high optical transparency combined with low electric resistivity, which allows their use as transparent contacts in photoelectric devices.[6–8] They are in particular promising for silicon-based solar cells with efficiency up to 22%.[6]

Substantial difference in electron work functions between silicon (Si) and most metal oxides (MOs) results in energy band bending, providing an enhanced separation of photogenerated charge carriers at the interface of MO/Si heterostructures. It has been already demonstrated for heterostructures with semiconducting oxides such as MoO_x,[8–14] VO_x,[15–17] WO_x,[18,19] NiO_x and TiO_x,[7,20,21] CuO_x, and[22,23] MoS_x[24] having bandgaps in the range of 3.0–3.8 eV and electron work functions between 4.5 and 6.5 eV.[24] Meanwhile, mechanisms of the charge carrier separation at the MO/Si interfaces and subsequent carrier transport through the MO layers have not been analyzed in detail.[9,14,25] Note that interband tunneling and trap-assisted tunneling are important mechanisms in the operation of the MO/Si heterostructures and have to be considered.[26]

In this article, we propose a model of an enhancement of charge carrier separation and their transport in heterojunction solar cells composed of a semiconductor (Sem) and metal oxide. The efficiency of the carriers separation is numerically estimated for MoO_x/n-Si heterojunctions and compared with available experimental data.

2. Model

2.1. Energy Bands

To enhance separation of charge carriers photogenerated in a heterojunction solar cell, it has to have an active region with the energy bands shown in **Figure 1**.

The semiconductor where charge carriers are mainly photogenerated is indicated as Sem and MO stands for the semiconducting metal oxide enhancing extraction of holes from Sem. The materials have to meet the following requirements. MO is a wide-bandgap semiconductor ($E_g > 2.5$ eV) as much as possible so that it is transparent to the incident sunlight, with intrinsic or light n-type conductivity and hole traps (E_t) in the bandgap. Sem is a small- or medium-bandgap semiconductor ($E_g < 1.5$ eV) with n-type conductivity effectively absorbing the sunlight. Electron work function in the MO has to exceed that in Sem. A thin conducting light transparent metallic film Me

A. L. Danilyuk, T. N. Sidorova, V. E. Borisenko
Department of Micro- and Nanoelectronic
Belarusian State University of Informatics and Radioelectronics
P. Browka 6, Minsk 220013, Belarus

V. E. Borisenko
Institute of Nanotechnologies in Electronics, Spintronics and Photonics
National Research Nuclear University MEPhI
Kashirskoe Shosse 31, Moscow 115409, Russia

H. Wang, R. Rusli, C. Lu
School of Electrical and Electronic Engineering
Nanyang Technological University
Singapore 639798, Singapore
E-mail: clu010@e.ntu.edu.sg

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