Formation of MoO_3/n-$BaSi_2$ heterojunctions for solar cell applications

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Introduction Recently, thin-film solar cells such as Cu(In,Ga)Se_2, Cu_2ZnSnS_4, and CdTe have been attracting so much attention due to their high efficiency and low cost. Barium disilicide ($BaSi_2$) might be another candidate material for thin film solar cells. The band gap of $BaSi_2$ is approximately 1.3 eV, which matches the solar spectrum better than crystalline Si. $BaSi_2$ also has a large absorption coefficient of over 3×10^4 cm^{-1} for photon energy greater than 1.5 eV. We have already grown high-quality $BaSi_2$ epitaxial layers on both Si(111) and Si(001) substrates even though $BaSi_2$ has an orthorhombic crystal structure. The undoped n-$BaSi_2$ has a large minority-carrier (holes) diffusion length (~10 μm) and thereby a long minority carrier lifetime (>10 μs). In our previous works, we have already achieved large photocurrent corresponding to the internal quantum efficiency exceeding 70% for the 400 nm-thick undoped n-$BaSi_2$ layer grown on the Sb-doped n^+-$BaSi_2$/p^+-Si TJ. These results have suggested that $BaSi_2$ is a very promising material for thin-film solar cell applications. Recently, transition metal oxides such as MoO_3, NiO, W_2O_5, have been widely used in organic solar cells as electron or hole transport layers. In this work, we formed a MoO_3/n-$BaSi_2$ heterojunction solar cell in which the MoO_3 layer works as the hole transport layer. Electrical and optical properties have been investigated.

Experimental After cleaning the n^+-Si substrate (ρ < 0.01 Ω·cm) at 900 °C for 30 min in high vacuum chamber, firstly a thin $BaSi_2$ template layer was grown by reactive deposition epitaxy at 500 °C. After that, an approximately 600-nm-thick undoped n-$BaSi_2$ layer was grown by MBE at 600 °C for 8 h. After the growth, the sample was taken out from the vacuum, so the surface of the sample was a little oxidized. Then another 15-nm-thick MoO_3 layer was deposited on the undoped $BaSi_2$ layer by vacuum evaporation. Finally, 1-mm-diameter ITO electrodes were deposited on the front side of the sample by RF-sputtering. Back contacts were formed by Al sputtering.

Results and discussions Figure 1(a) shows the *J-V* characteristics of the sample under dark and illumination (AM1.5) conditions at room temperature. Clear open circuit voltage and short circuit current density have been obtained from this heterojunction solar cell. Although both of them are still very small, they give a strong evidence that $BaSi_2$ is a good candidate for thin film solar cells. Figure 1(b) shows the quantum efficiency spectrum of the sample. From the spectrum, the quantum efficiency increases quickly for photon energy large than 1.3 eV, which matches the band gap value of $BaSi_2$ very well from our previous works. The notch at about 2.5 eV in the spectrum is caused by the interference of the transparent ITO and MoO_3 layers. Figure 1(c) shows the quantum efficiency of the sample under reverse bias voltages. Quantum efficiency increases dramatically when reverse bias voltages are added to the sample, which indicates that the build-in electrical field stretches effectively in the undoped $BaSi_2$ layer. We speculate that the reason of this phenomenon is the short minority carrier lifetime or the high carrier density of the undoped $BaSi_2$ layer.

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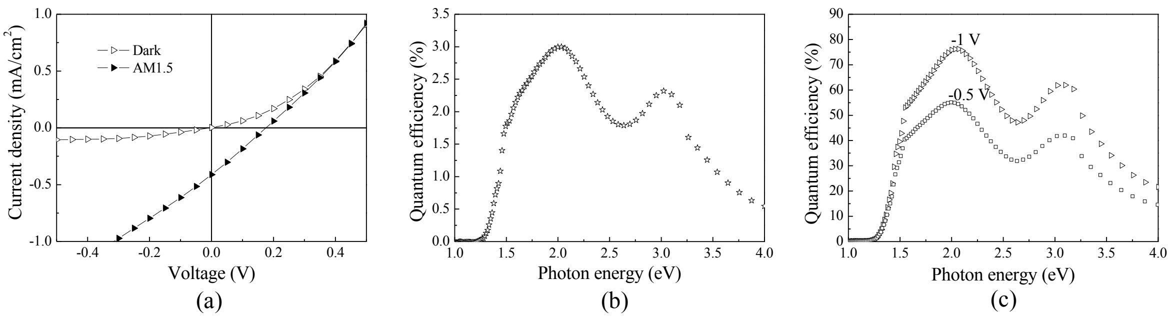

Fig 1 (a) *J-V* characteristics of the sample measured under dark and illumination (AM1.5) conditions, (b) Quantum efficiency spectrum of the sample, (c) Quantum efficiency spectrum of the sample under reverse bias voltages.