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I-V and C-V characteristics of the metal/undoped-BaSi₂ Schottky diodes

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<u>Introduction</u> Recent years, thin film solar cells have been paid more and more attention due to its high efficiency and low cost. Barium disilicide $(BaSi_2)$ is a new kind of semiconducting material with lots of excellent features. The band gap of $BaSi_2$ was found to be about 1.3 eV. Both theoretical and experimental

researches have revealed that BaSi₂ has a very large absorption coefficient of approximately 3×10^4 cm⁻¹ at 1.5 eV. High-quality BaSi₂ films can be grown on both Si(111) and Si(001) substrates. However, due to the large band offset at BaSi₂/Si interface (~0.6 eV), we need to firstly grow a tunnel junction (TJ) on low-resistivity Si substrates, then a BaSi₂ *pn* junction diode on the TJ. In our previous works, over 90% internal quantum efficiency has been achieved on a 1.2-µm-thick undoped BaSi₂ layer grown on an n⁺-BaSi₂/p⁺-Si tunnel junction, showing that BaSi₂ is a very promising candidate for high-efficiency thin-film solar cells.¹⁻³⁾ In this work, Schottky junctions were formed on the thick undoped BaSi₂ layers grown on TJ, and the *I-V* and *C-V* characteristics were measured.

Experiment After cleaning p⁺-Si ($\rho < 0.01 \ \Omega \cdot cm$) substrates at 900°C for 30 min, firstly a thin BaSi₂ template layer was grown by RDE at 500°C, then an approximately 30-nm-thick Sb-doped n⁺-BaSi₂ layer was grown at 550°C by MBE for 20 min. After that, about 1150-nm-thick undoped BaSi₂ layer was grown by MBE for 15 h at 600°C. After the growth, the sample was cut into pieces and treated for RTA at 750°C for 30 s. 1-mm-diamter Au/Cr surface electrodes (A = 7.85×10⁻³ cm²) were formed on both as-grown and RTA-treated samples by vacuum evaporation. Backside electrodes were also formed by Al evaporation.

Results and discussions Figure 1 shows the I-V characteristics of (a) as-grown and (b) RTA-treated samples. Clear rectifying properties were observed in both samples, indicating that the Schottky junctions were formed successfully on the surface of the thick undoped $BaSi_2$ layers grown on the TJ. The blue-colored I-Vcurves, in which the series resistance and shunt resistance were subtracted, were also plotted. The logarithmic plots of current density J with respect to V are shown in Fig. 2. The reverse saturation current density J_s can be extracted from the straight line intercept of Ln(J)-V plot at zero bias voltage. J_s was 2.88×10^{-4} A/cm² for as-grown sample and 1.43×10^{-5} A/cm² for the sample treated by RTA, respectively. For a Schottky junction, from the thermionic emission theory, $J_s = A^*T^2 exp(-q\phi_s/KT)$, here A^{*} is effective Richardson constant, ϕ_s is the barrier height at zero bias. ϕ_s were calculated to be 0.62 and 0.70 V, respectively. Figure 3 shows the characteristics of $1/C^2$ vs. reverse bias voltage V plots. The build-in potential can be deduced by extending the linear curve to the voltage axis. The built-in potential was 0.53 V for the as-grown sample and 0.62 V for the sample treated by RTA. In both samples, the carrier densities of undoped n-BaSi₂ were on the order of 10¹⁶ cm^{-3} .

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Fig. 1 *I-V* characteristics of (a) as-grown and (b) RTA-treated samples.



Fig. 2 Ln(I) vs. V characteristics for the asgrown and RTA treated samples.



Fig. 3 $1/C^2$ vs. V plots for the as-grown and RTA treated samples.