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Investigation of the temperature dependences of the I-V characteristics of p-Si/MoO_x selective contacts

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Abstract. In this article the temperature dependences of selective contacts based on MoO_x were studied. The p-Si/MoO_x/Al structure was fabricated. Current-voltage and capacitance-voltage characteristics in the temperature range from 80 to 300K were measured. Band diagram was also calculated to reveal potential barriers location and its influence on charge carrier transport.

1. Introduction

In the manufacturing of semiconductor devices electrical contacts play an important role. The optimal contact should have a minimal effect on the properties of the device's structure and at the same time have an ability to freely pass charge carriers into an external circuit. In the case of a semiconductor device operating in a wide temperature range the electrical contact must also maintain its characteristics.

Currently, there is growing interest in the use of renewable energy sources, including solar energy as an alternative to conventional sources such as oil, coal and gas. The main direction of photovoltaics is the development of new configurations of solar cells (SC) in order to increase efficiency, as well as to reduce their cost. The cost of modern solar cells is almost 50% determined by the cost of the substrate. In this case, silicon-based SCs (mono- and polycrystalline) are currently most widely used. Further, the cost of solar cells is strongly influenced by energy costs for technological processes. For example, for a long time, silicon SCs were manufactured by high-temperature diffusion of phosphorus into p-type silicon, after which a back contact was formed based on the burning of aluminum at a temperature of 600-700 ° C. All this requires significant energy costs.

Recently, in photovoltaics there has been a shift towards low-temperature approaches in the manufacture of solar cells. Due to the development of plasma chemical deposition methods, silicon heterojunction solar cells are widely used. During their manufacture, thin layers of amorphous hydrogenated silicon (a-Si:H) are deposited onto the surface of a silicon substrate at temperatures not exceeding 250 °C. In this case, an a-Si:H/Si heterojunction is formed, which also plays a role in decreasing the surface recombination rate of charge carriers at the interface and, as a result, the open circuit voltage of the solar cells increases.

At the same time, due to the significant absorption of short-wave solar radiation in amorphous silicon, the short-circuit current of such SCs is still not high enough. Recently, there has been growing interest in systems of materials with selective properties with respect to transport of charge carriers of a certain polarity, in particular, to carrier-selective contacts [1,2]. For example, in [3] it was shown

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that selective contacts based on molybdenum (VI) oxide can be successfully used in the manufacture of solar cells, while the efficiency already reaches 18%. Moreover, MoO₃ has an absorption coefficient in the short-wavelength region of the solar spectrum several orders of magnitude less than a-Si:H [4], which makes it a promising material for use in highly efficient solar cells.

It is known that parameters of solar cells are measured at a temperature of 25 °C; however, their operation can also be carried out at lower temperatures. In this case, the band structure parameters are changing, in particular, at the Si/selective contact interface. Due to the principle of the selective contact operation, even insignificant changes in the Fermi level in silicon due to the temperature lowering can lead to a significant increase in the potential barrier for charge carriers. Thus, the goal of this work was to study the features of carrier transport through selective contacts based on molybdenum oxide for p-type Si over a wide temperature range.

2. Experimental details

In this work selective contacts were fabricated for p-type double side silicon (100) wafers made by Czochralski method. Measured by the Hall method acceptor concentration in p-type silicon was $2 \cdot 10^{16}$ cm⁻³. Before making the contacts, the surface layer of SiO₂ was etched in the hydrofluoric acid solution (1:10). Then the samples were immediately placed in a vacuum chamber.

To study the transport properties of selective contact for p-Si, a symmetric Al/MoO_x/p-Si/MoO_x/Al structure was made. MoO_x means that during the thermal deposition process some oxygen atoms reacts with vacuum chamber and thus the material is not stoichiometric. First, 30 nm of molybdenum oxide (VI) was thermally evaporated on the top silicon surface through a metal mask with 0.6 mm diameter holes. Next, Al contact (200 nm) was sputtered onto MoO_x layer by magnetron deposition in Boc Edwards Auto 500 vacuum chamber. Back contact was formed in the same way but without metal mask (Figure 1).



Figure 1. Schematic of p-Si/MoO_x/Al structure.

Standard I-V curves were measured using a Keithley 2400 source-meter and Janis VPF 100 liquid nitrogen cryostat providing measurements in the temperature range of 80–300 K. Admittance was measured using an Agilent E4980A precision LCR meter.

3. Experimental results

Figure 2a shows the current – voltage characteristics of the contact based on p-Si/MoO_x/Al, depending on the temperature from 80 to 300 K, plotted in semi-logarithmic coordinates. Lowering the temperature leads to currents decrease. In the range of 250 K to 300K I-V curves exhibit a liner behavior, while at the lower temperature a non-linear behavior is observed. The temperature dependence of the current density at an applied voltage of -1.5 V is presented in Figure 2b. The current density has a weak temperature dependence in the range of 300- 250 K, while in the 100-200 K range it exhibits an exponential dependence with an activation energy of about 0.05 eV.

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Figure 2. MoO_x/Al based contact I-V characteristics (a) and current values at -1.5V (b) as a function of temperature.

Nevertheless, in absolute value, the current density passing through the p-Si/MoO_x/Al contact at room temperature significantly exceeds typical currents in solar cells, where they usually do not exceed 40 mA/cm². Even at the temperature of 80 K, current value at a voltage of -1.5 V reaches 250 mA/cm².

To study the nature of the temperature behavior of the current density, the capacitance-voltage characteristics of this contact were measured. Figure 3a shows the dependence of the capacitance of the selective $p-Si/MoO_x/Al$ contact on the applied voltage, measured at different temperatures. In all cases, a decrease in capacitance is observed with an increase in the applied reverse voltage. Also, a decrease in capacity occurs with a decrease in temperature (Figure 3b).



Figure 3. Graph of capacitance versus applied voltage (a) and capacitance values at 0 V (b) as a function of temperature.

Figure 4a shows the dependence of capacitance on voltage in the Mott-Schottky coordinates. It can be seen from the graph that there are several linear sections, the slope of the curves varies with temperature, so it is quite difficult to calculate the value of the flat band potential in the framework of the classical theory. However, the general trend of the capacitance decreasing with applied voltage as well as strong capacitance increase with temperature could indicate a presence of potential barrier. Further detailed studies should be carried out, in particular by applying admittance spectroscopy, to distinguish between potential barrier and defect response input into capacitance.

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Figure 4. Capacitance versus voltage in Mott-Schottky coordinates.

To explain the behavior of the I–V characteristics with temperature, we calculated the band diagram of the p-Si/MoO_x/Al system shown in Figure 5. The band gap of 3 eV and electron affinity of 6 eV for MoO_x layer were used according to Ref. [5] and [6], respectively.



Figure 5. Band diagram of the p-Si/MoO_x/Al structure.

Oxygen vacancies in reduced MoO_x (x < 3) acts as donor impurities shifting its Fermi level closer to the conduction band [6]. A significant energy barrier for electrons in p-Si is formed at the p-Si/MoO_x heterointerface (Figure 5), which limits their transport through the interface and, therefore, suppresses surface recombination. On the other hand, holes transport through the p-Si/MoO_x interface is provided by recombination with electrons in MoO_x due to direct band to band tunneling or trap assisted tunneling (multitunneling capture emission) [7]. Thus, an effective selective contact for the holes is achieved. However, a potential barrier for the electrons formed at the Al/MoO_x interface (Figure 5) could limit their transport at low temperature. Indeed, the observed non-linear behavior of I-V curves for low temperature range (100-250 K), as well as exponential current density temperature dependence confirm the formation of the potential barrier. For higher temperature (T > 250 K) the

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current density becomes to be limited by hole transport via $p-Si/MoO_x$ interface. The temperature dependence of this transport provided by tunneling is much weaker.

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