Temperature dependence of I-V characteristics in p-Si/MoO_x and n-Si/LiF/Ta selective contacts

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Abstract. The temperature dependences of I–V characteristics of structures with selective contacts based on molybdenum oxide and lithium fluoride were explored. p-Si/MoO_x and n-Si/LiF/Ta model symmetrical structures were made. It was shown that the operating current decreasing with temperature decreasing to the one of liquid nitrogen.

1. Introduction
In the production of semiconductor devices, the fabrication of electrical contacts is one of the most important tasks. The main characteristic of electrical contact is contact resistance. It determines the electric potential drop at the contact when an electric current passes through it. So, during the operation of the solar cell (SC), even a small potential barrier at one of the contacts can significantly reduce the conversion efficiency of solar radiation. Besides the contact resistance, it is important to take into account such a parameter as the rate of surface recombination at the semiconductor/contact interface in the production of solar cells. Photogenerated charge carriers move towards the contacts under the light in a solar cell, however some of them recombine at this interface without reaching the external circuit due to the high surface recombination rate.

The first contacts to solar cells were formed by burning metals into a semiconductor. However, due to the high recombination at the contact in this case, the open circuit voltage of such SCs was low. Moreover, this technology requires high temperatures, which affects the cost of the solar cells.

Recently, a low-temperature approach to the fabrication of solar cells has been rapidly developed. Plasma-chemical methods for the formation of layers with a few nm thicknesses, which play the role of both passivating layers and the role of highly doped layers, are increasingly used. With this approach, the contact layer is usually either a transparent conductive oxide or a metal layer with a low resistivity. This type of solar cells reaches a record efficiency of about 26% in silicon single-junction one [1]. A further increase in efficiency requires the improvement of technology and the development of new approaches. For example, in common heterojunction SCs based on crystalline/amorphous hydrogenated silicon (c-Si/a-Si:H) a part of the solar radiation is absorbed in the a-Si:H layer. Its replacement by wide bandgap semiconductor can increase short-circuit current leading to increase the efficiency of such solar cell.

Recently, there has been growing interest in systems of materials with selective properties with respect to the transport of charge carriers of a certain sign, in particular, to selective contacts [2, 3].
For example, it was shown that selective contacts based on molybdenum oxide can be successfully used in the fabrication of solar cells, while the efficiency reaches 18% in [4].

As known, efficiency of solar cells was measured at 25 °C; however, their performance can also be carried out at temperatures below zero, while the parameters of the band structure of the silicon/selective contact system change. Due to the principle of the selective contact operation [5], even small 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. The aim of this work is to study carrier transport through selective contacts based on molybdenum oxide and lithium fluoride for silicon substrates of various doping levels and types of conductivity in the wide temperature range.

2. Experiment details
In this work, selective contacts were fabricated for p- and n-type double side silicon (100) wafers produced by Czochralski method. Doping of p-type silicon of $2 \cdot 10^{16}$ cm$^{-3}$ was measured by the Hall method while for n-type silicon it was $1 \cdot 10^{15}$ cm$^{-3}$. Before contacts fabrication, the surface layer of SiO$_2$ 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 formed. First, 30 nm of molybdenum oxide (IV) 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. Bottom contact was formed in the same way but without metal mask (see figure 1a).

![Figure 1. Schematic view of structures (a) – for p-type Si; (b) – for n-type Si.](image)

Selective contact for n-type silicon wafer was formed by thermal evaporation of lithium fluoride (5-10 nm) through a metal mask with 0.6 mm diameter holes. Ta contact (200 nm) was sputtered onto LiF layer by magnetron deposition. The difference in structures for the second one is difficulties in thermal deposition of LiF film with reproducible thickness. Here it is very important since thicker back contact can limit measured current.

Standard I-V characteristics were measured using a Keithley 2400 source-meter in Janis VPF 100 liquid nitrogen cryostat providing measurements in the temperature range of 80–300 K.

3. Results and discussion
I-V characteristics of MoO$_X$ and LiF based selective contacts were measured at different temperatures (see figure 2). For the contact to p-Si all curves demonstrate high current down to the temperature of 80 K. The difference in absolute current values in the temperature range of 80-300 K is about 2 orders.
Figure 2. I-V characteristics of the contacts based on p-Si/MoO$_x$/Al (a) and n-Si/LiF/Ta (b) measured at different temperature (plotted in semi-logarithmic scale).

For the LiF-based selective contact to n-type silicon the difference in current values measured at 80K and 300K is about four orders. It is important to note that the I-V curves were measured in “top-top” mode. In this case, LiF film thickness is the same in both contacts and thus the contact properties are also have to be equal. On the other hand, the distance between two contacts is much higher, therefore, it is necessary to keep in mind the temperature dependence of silicon resistivity. According to the measurements being provided in [6] changes in silicon resistivity in a temperature range of 80-300 K are no more than 10 times. Consequently, the demonstrated in figure 2b I-V curves behavior is more related to the contact characteristics changes.

To explain the behavior of the I-V characteristics versus temperature, the band diagrams of the p-Si/MoO$_x$/Al and n-Si/LiF/Ta were calculated, and they are shown in figure 3. The band gap of 3 eV and electron affinity of 6 eV for MoO$_x$ layer were used according to Ref. [7] and [8], respectively. For the lithium fluoride the band gap of 13.6 eV [9] and electron affinity of 1.8 eV [10] were used.

A significant potential barrier for electrons in p-Si is formed at the p-Si/MoO$_x$ heterointerface (see figure 3a). On the other hand, holes transport through the p-Si/MoO$_x$ interface is not restricted. For the n-type Si electron transport is realized via tunneling throw the thin dielectric layer (LiF). Band bending is determined by metal work function, and in case of Ta (4.2 eV) it is presented in figure 3b. Due to low film thickness, electrons tunnel through the barrier, whereas, the holes are moved out by the electric field. In the both cases the rate of surface recombination is decreased drastically and this effect also could be used in solar cells contacts manufacturing.

High current values on I-V curve for p-Si/MoO$_x$/Al at 300K is explained by the band diagram, whereas the current values for the n-Si/LiF/Ta are in two orders lower due to tunneling restrictions. However, a potential barrier for the charge carriers formed at the interface contacts could limit their transport at low temperature. Figure 4 shows the difference in I-V curves for the investigated contact systems measured at room temperature and at 80K. In absolute value, the current density passing through the p-Si/MoO$_x$/Al contact at room temperature significantly exceeds typical current in solar cells which is usually lower 40 mA/cm$^2$. Even at the temperature of 80 K, current value at a voltage of -1.5 V reaches 250 mA/cm$^2$. 
Figure 3. Band diagrams of the p-Si/MoO\textsubscript{x}/Al (a) and n-Si/LiF/Ta (b) structures.

Figure 4. I-V characteristics of the contacts based on p-Si/MoO\textsubscript{x}/Al (a) and n-Si/LiF/Ta (b) measured at 300 K and 80 K (in the inset).

Absolute current values measured for the n-Si/LiF/Ta system are in 2 orders lower then for the p-Si/MoO\textsubscript{x}/Al contact, but they may still be applied in solar cells operated at room temperature. However, at low temperatures there is a sharp drop in current values is observed that makes this type of contact is not suitable to be as a part of solar cells.

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