Nanostructured Heterojunction Crystalline Silicon Solar Cells with Transition Metal Oxide Carrier Selective Contacts

One of the most severe challenges man is facing today is to satisfy the need for energy without harmful environmental consequences. This complicated, grand challenge must be met by a wide range of solutions; among these are more efficient use of resources and replacement of fossil fuels by renewable energy sources. Any sustainable, renewable energy system must directly or indirectly rely on solar energy. Photovoltaic or solar cells are already efficient and reliable sources of electricity from solar light, but even though their cost has decreased significantly in recent years, solar cells are still far too costly for a competitive production of bulk grid power. The challenge within the solar cell field is thus to reduce the costs involved in solar cell production without sacrificing efficiency and reliability; actually, the efficiency should better improve towards 25 % or more, since the cell efficiency strongly affects the overall economy of a solar cell power plant. Currently, most of the solar cell market is based on 180-300 micrometer thick crystalline silicon wafers, and approximately 50 % of the cost is due to the cost of the material. To reduce material costs, introducing thin-film cells is a promising alternative, but a limitation in thin film solar cell technologies is that the absorptivity of light is quite weak, in particular for indirect band gap materials like silicon. This limitation may be lifted by application of photon trapping strategies that can increase the absorptivity of thin photo-absorbers by orders of magnitude at longer wavelengths. Another proven approach in solar cell optimization is carrier selective contacts, such as conventional amorphous silicon, or wide bandgap metal oxide semiconductor.

In this Ph.D. thesis, I present several new ideas for novel silicon-based solar cells to develop efficient solar cells that can be fabricated in a low thermal budget, and with the low-cost fabrication procedure using only abundant ecocompatible materials. The main photo-absorber is lightly doped p-type silicon (1.12 eV band gap) with a thin n-type TiO$_2$ (3.2 eV band gap) film on top. This structure forms a p-n heterojunction that effectively separates the photogenerated electron hole-pairs since the TiO$_2$ and silicon conduction bands are aligned facilitating electron transport, while a 2 eV valence band energy barrier prevents hole transport. The electrons transported in the conduction band through the TiO$_2$ to the surface are conducted laterally by a metal grid or continuous transparent conductive oxides (TCO) such as Aluminum Zinc Oxide (AZO) with high conductivity, highly transparency (optical losses 10%) electrode layer. On the backside, silicon was coated with complementary to TiO$_2$ thin film of NiO. NiO is a p-type wide bandgap (3.6 eV) semiconductor. In connection to silicon it forms a p-p isotype heterojunction with excellent valence band matching and creating hole conducting and electron blocking layer. As a back contact, I used high work-function metals to form an additional potential barrier against electron transport, while the holes could easily conduct to the metal. This basic structure was combined with micro- and nanostructuring of the silicon surface prior to fabrication to reduce optical reflectance below 1 % and to enhance light trapping inside the absorber layer. All fabrication procedures were completed at temperatures close to room temperature with a maximum of 200 °C in a single step, and thus the thermal budget became unusually low.

The overall Ph.D. thesis project had four main research phases. In the first phase, the basic TiO$_2$-Si heterostructure was investigated on planar silicon wafers. Here, I focused on development and optimization of fabrication procedures for obtaining excellent TiO$_2$ passivation quality, high-performance junctions and efficient lateral transport. In addition, I found that the atomic layer of Al$_2$O$_3$ between TiO$_2$ and silicon enhanced passivation properties and junction performance. Using atomic layer deposition (ALD) techniques, thickness and material composition of TiO$_2$ and Al$_2$O$_3$ were highly precisely controlled. The fabricated test structures of TiO$_2$ and Al$_2$O$_3$ showed high open circuit voltage $V_{OC}=0.63$ V) and short-circuit current $J_{SC}=20$ mA/cm$^2$. Other metals with close by work function (Al, Ti, Ni) were tested to minimize current blocking effects in diode structure. In the second stage, NiO-Si isotype heterostructure was tested and optimized to meet the best ohmic (hole conductive) properties. I fabricated and characterized NiO-Si structure similar to the TiO$_2$-Si structure. Using sputtering from NiO target and ALD techniques, I obtained conformal NiO films with excellent ohmic behavior but modest passivation quality. Next stage, I optimized nanostructuring process for silicon surfaces with reactive ion etching (RIE) and obtained a so-called black silicon. Using low surface damage RIE strategy, nanostructured surfaces I obtained low reflectivity (1 %) and surface recombination velocity (SRV4 cm/s) in comparison to KOH-textured and plane silicon. Black silicon nanostructured surfaces were passivated with ALD Al$_2$O$_3$ grown at 200 °C and annealed at 400 °C.

Finally, after the previous three stages were completed, I applied our process development results in HIT-type architecture on the recent record silicon solar cell type. However, due to a combination of many new concepts the fabricated solar cells did not show excellent performance and needed further investigation and optimization.

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