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In this thesis, novel optically-rough and physically-flat transparent conductive oxide (TCO) substrates were developed for thin-film solar cells with superstrate configuration. These substrates consist of a widegap Zn$_{1-x}$Mg$_x$O transparent conductive thin film prepared by sol-gel process and glass substrates with rough surfaces prepared by reactive ion etching or nano-imprinting technique.

Firstly, Zn$_{1-x}$Mg$_x$O thin films with wide bandgap and low resistivity were developed by sol-gel process. Resistivity of about $3.9 \times 10^{-3}$ $\Omega \cdot$ cm was achieved for a sol-gel Zn$_{1-x}$Mg$_x$O thin film with an optical bandgap of 3.61 eV (Mg/Zn=10 mol. %, thickness=681 nm). Al doping contributed to the decrease in resistivity and the increase in optical bandgap. Annealing atmosphere in two-step annealing process played an important role in improving the electrical and optical properties of Al-doped Zn$_{1-x}$Mg$_x$O (AZMO) thin film. It was found that the first step annealing in nitrogen increased carrier concentration, and the second step annealing in forming gas with a glass cover contributed to the improvement of Hall mobility. An optimum H$_2$ concentration in forming gas existed for decreasing the resistivity of AZMO thin film when the second annealing in forming gas was conducted without glass cover. This sol-gel AZMO thin film enables “physically-flat” concept on roughened substrates.

Secondly, conditions of reactive ion etching (RIE) of glass substrates and shapes of imprinting patterns were investigated in details to realize a scattering interface for fabricating “optically-rough” structure. In the part of RIE, moderate feature size on the substrate was obtained by controlling the etching time, RF power of plasma generation, and pressure. The etched Corning XG glass showed larger vertical feature than the etched 7059 glass, resulting in large haze ratio at long wavelength. After coating sol-gel AZMO thin film with 2-methoxyethanol as solvent, the AZMO/RIE etched 7059 glass substrate showed smooth surface and good scattering behavior. In the part of room-temperature nanoimprinting, the shape and period of feature size on the patterned substrate influence the optical properties of substrates greatly. Substrates imprinted with hole and pillar patterns showed high haze ratio at long wavelength region, indicating good light-scattering behavior. After AZMO coating, the AZMO/glass substrate patterned with a hole pattern showed a flat surface and a high haze ratio at long wavelength region. In terms of overall performance, the AZMO/hole patterned substrate shows high haze ratio and low surface roughness. AZMO(0.75 M 40L Mg/Zn=10
mol. %)/substrate with a hole pattern (period=1.7 μm) showed a root-mean-square surface roughness of 2.6 nm, a sheet resistance of 47.0 Ω/sq, and an average haze ratio of 9.5% at wavelength region from 700 nm to 850 nm. This value was larger than that of the typical ZnO·B substrate with pyramidal surface morphology, which was deposited by the metal organic chemical vapor deposition method.

Subsequently, these AZMO substrates were applied as the transparent conductive layer in hydrogenated amorphous silicon solar cells (a-Si) single junction solar cells with superstrate configuration. Bandgap widening of TCO through increasing Mg content improved the spectral response at short wavelength, however, too wide bandgap (E_{opt} >3.55 eV) deteriorated the performance of solar cells due to the decrease in J_{sc}, V_{oc}, and FF. Solar cells deposited on AZMO (E_{opt}=3.55 eV, Mg/Zn=10 mol. %)/flat glass substrate showed the best performance. Employing 20 nm Nb-doped TiO_{2} thin film as the antireflection layer at the TCO/p-a-SiC_x interface improved the spectral response of a-Si solar cells at wavelength of 450-580 nm through reducing the optical reflection. Roughening surface morphology of AZMO thin film via utilizing the nonequilibrium solute precipitation and crystallization process during the drying procedure improved the spectral response of a-Si solar cells at wavelength of 600-800 nm by enhancing the light-scattering, however, deteriorated the overall performance. When the optically-rough and physically-flat AZMO substrate was applied as the front electrode of a-Si single junction solar cells, the spectral response at short wavelength of around 350 nm was improved obviously due to the decrease in optical loss. A high \( V_{oc} \) of 0.92 V was obtained by using AZMO/RIE etched 7059 (7 Pa 250 W 10 min) glass substrate due to the flat surface. A solar cell with \( \eta \) of 8.02 % (\( V_{oc}=0.88 \) V, \( J_{sc}=13.02 \) mA/cm\(^2\), and \( FF=0.70 \)) was obtained by using AZMO/RIE etched 7059 glass substrate (7 Pa 200 W 10 min). A \( J_{sc} \) of 13.2 mA/cm\(^2\) was achieved with AZMO(40L)/hole (period=1.7 μm) patterned substrate.

Overall, a novel optically-rough and physically-flat AZMO substrate was developed. This substrate showed low optical absorption, low surface roughness, high haze ratio in transmission at long wavelength region, and moderate sheet resistance, simultaneously. It was demonstrated that a-Si single junction solar cells fabricated on this substrate showed good device performance. These results indicate the potential of the optically-rough and physically-flat AZMO substrate for the front electrode of several types of thin-film solar cells.