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Thermally Stable Hole-Selective Zn-doped NiO_x Deposited onto Crystalline Silicon

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Transition metal oxides (TMOs) have attracted enormous interest as novel passivating contacts for silicon solar cells. Among various TMOs, molybdenum oxide (MoO_x), tungsten oxide (WO_x) and vanadium oxide (VO_x) are the most widely studied materials which showed hole-selectivity in contacts with Si. They tend to have oxygen vacancies which make them *n*-type semiconductors. When contacting with Si, their high work function (~ 6 eV) helps induce band bending in Si and align the Fermi level close to the valence band, which facilitate the hole extraction. Unlike these three TMOs, nickel oxide (NiO_x) is intrinsically *p*-type because of Ni vacancies. It has a large band gap and small valence band offset with Si, which could provide a near-perfect band alignment for the extraction of holes in silicon. There are reports showing that the incorporation of Al, Zn, and Cu as dopants into NiO_x can alter the electrical and optical properties of NiO_x[1,2]. However, the application of these doped NiO_x in Si solar cells is yet to be reported. Predicted by the density functional theory (DFT) calculations, this work investigated zinc doped nickel oxide, $Zn_xNi_{1-x}O$ (ZNO) deposited by atomic layer deposition (ALD) and used as a potential passivating hole contact for Si. In addition, thermal stability of the hole-selective ZNO contacts is also studied as the fabrication of Si solar cells typically involves high-temperature processes.

Using the ALD super cycles, ZNO was deposited from diethylzinc (DEZ), bis(N, N'-di-t-butylacetamidinato) nickel(II) (NiAMD) and water. The $Zn_xNi_{1-x}O$ with different doping ratios, *i.e.*, x = 0.018, 0.05, 0.1 were investigated. The doping ratio is defined by the ratio of ZnO and NiO ALD cycles rather than the exact atomic ratio. Spectroscopic ellipsometry reveals that the deposited ZNO films have high optical transparency with a bandgap of > 4 eV. In Figure 1, the valence band spectra from X-ray photoelectron spectroscopy of bulk Si and the ZNO on Si are shown. The valence band offsets (VBOs) between the $Zn_xNi_{1-x}O$ (x = 0.018, 0.05, and 0.1) and Si are determined to be -0.33 eV, -0.64 eV and 0.36 eV, respectively[3,4]. Considering the bandgap energies of 1.12 eV and > 4 eV for the Si and the $Zn_xNi_{1-x}O$ respectively, the conduction band offsets between the ZNO films and Si are much higher than the VBO. Therefore, the ALD-deposited $Zn_xNi_{1-x}O$ (x = 0.018, 0.05, and 0.1) films should work effectively as a hole-selective contact for the Si. The contact performance measured by using the Cox and Strack method[5] showed that all the as-deposited ZNO films formed a good ohmic contact with the *p*-Si. In addition, while subsequent annealing at 200-500 °C significantly decreased the contact resistivity, post-treatment at these high temperatures did not degrade their performance (Figure 2). The best contact resistivity of ~21.5 $m\Omega \cdot cm^2$ is obtained by annealing the $Zn_{0.1}Ni_{0.9}O$ sample at 200 °C.

In conclusion, the material properties of the Zn doped NiO_x with different doping ratios made by ALD is analysed thoroughly. The ZnO films were observed to be thermally stable up to 500 °C. These thermally stable ZNO films deposited onto Si showed much potential as a hole-selective contact for the Si solar cells because of the unprecedented optical transparency as well as good ohmic contact with the Si.

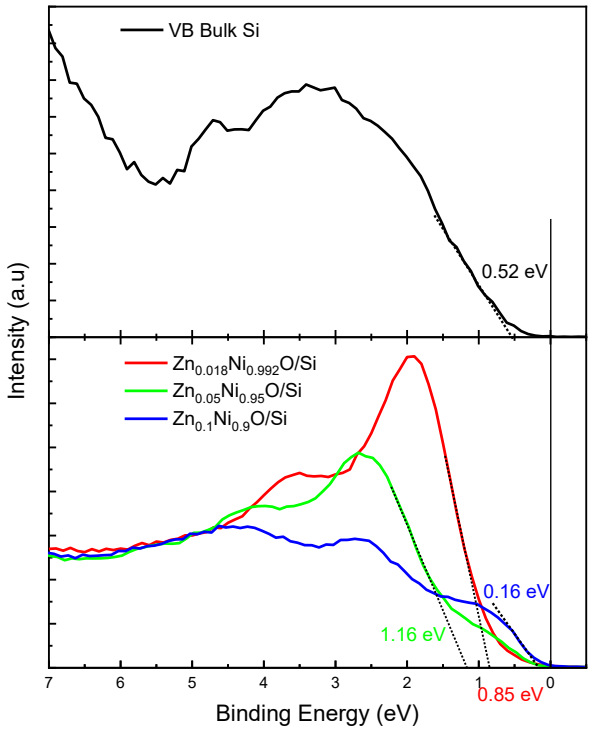

Figure 1. The valence band spectra of a bare Si and the $Zn_xNi_{1-x}O$ (x = 0.018, 0.05, 0.1) films deposited onto silicon substrate.

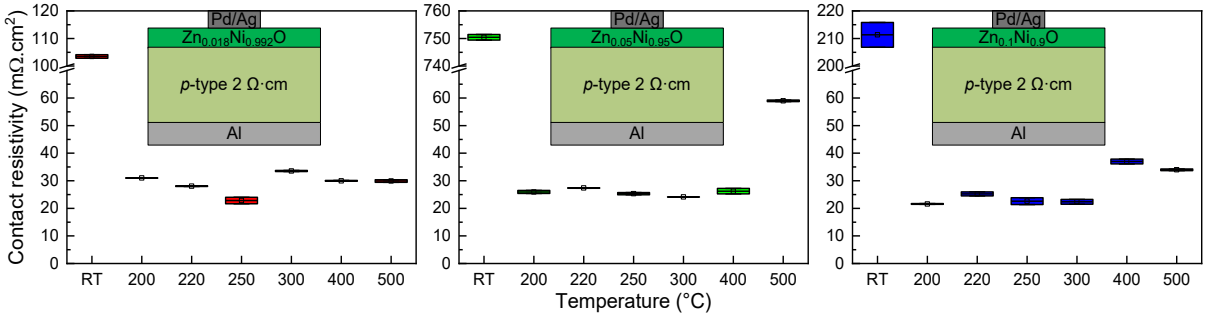

Figure 2. Contact resistivity of the $Zn_xNi_{1-x}O$ (x = 0.018, 0.05, 0.1) films onto p-Si before and after annealing.

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