

## **Investigation of Al<sub>2</sub>O<sub>3</sub> capping layers on MoO<sub>x</sub> and NiO<sub>x</sub> Passivating contacts via atomic layer deposition**

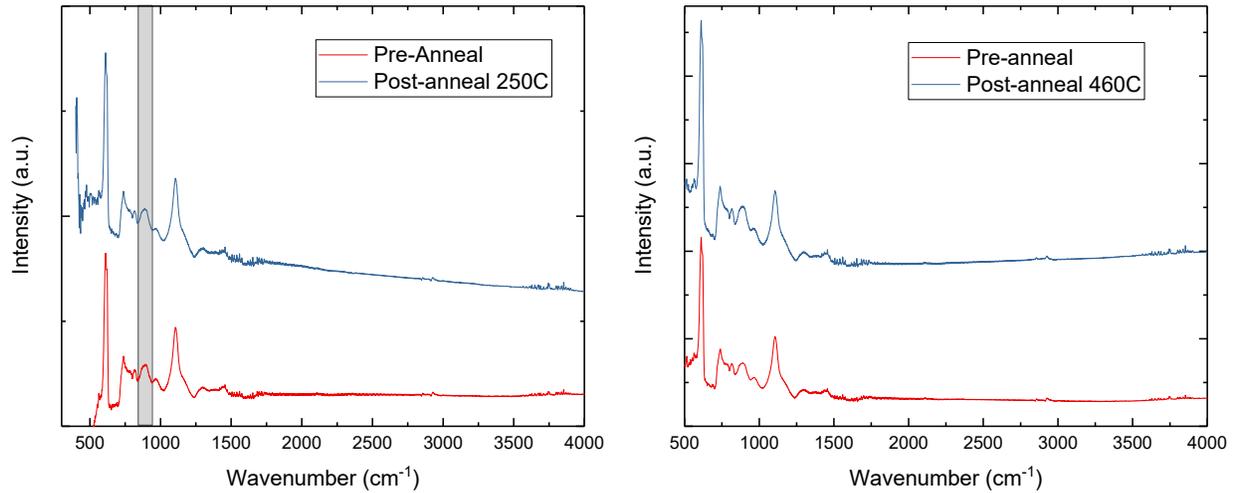
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Surface and contact passivation is an important aspect to consider when developing high-efficiency solar cells in particular when the solar cell thickness is further reduced. In recent years, there has been a lot of progress in this area in particular for passivating contacts where metal oxides are intensively investigated for both electron and hole passivating contact. One appealing method to synthesise these materials is atomic layer deposition (ALD). With a broad range of materials to work with, ALD has the benefit of precisely depositing highly conformal films into complex structures. It does this by utilising a binary sequence of half-reactions, ensuring one monolayer of growth per deposition cycle until the desired thickness is achieved. MoO<sub>x</sub> and NiO<sub>x</sub> are two materials that are studied as hole passivating contacts. These high work function metals contacts in combination with Si causes the Fermi level to bend towards the valence band of Si, where the film provides high conductivity for holes and low conductivity for electrons. This is critical for the selective extraction of charge carriers. MoO<sub>x</sub> and NiO<sub>x</sub> are metal oxides that are known to degrade due to exposure to the moisture in the ambient (Glen *et al.*, 2016), thus mandating an additional moisture barrier. It is known that Al<sub>2</sub>O<sub>3</sub> is ideal as a protective capping layer as it also enhances the passivation parameters post-annealing, with recent examples showing the a reduction of J<sub>0</sub> to 3.3 fA/cm<sup>2</sup> and a respectable implied open circuit voltage of 724 mV (Black and Kessels, 2018). This provides a great incentive to further investigate how Al<sub>2</sub>O<sub>3</sub> will improve the passivation quality of the hole passivating contacts.

280 um FZ *p*-type c-Si (1-5 Ωcm resistivity) wafers were first cleaned using the RCA1/2 process. These wafers were then HF dipped to remove existing oxide layers, resulting in a hydrogen-terminated surface. Using plasma-enhanced ALD, NiO<sub>x</sub> and MoO<sub>x</sub> were deposited on c-Si with thicknesses of 5 nm and 10 nm each. Half of the wafers were then capped with Al<sub>2</sub>O<sub>3</sub> using thermal ALD, which used trimethylaluminium (TMA) and H<sub>2</sub>O as precursors. The wafers were sent for a high temperature anneal for 10 min, with the annealing temperature ranging from 250 to 460 °C. To support this investigation, the electrical properties of the wafers were characterised using quasi-steady state photoconductance with a Sinton lifetime tester. Improvements in the passivation quality can be quantified from the J<sub>0</sub> and lifetime value, where the investigation aims to achieve J<sub>0</sub> values below 100 fA/cm<sup>2</sup>. For the changes in material properties, Fourier-transform infrared (FTIR) was used to detect vibrational modes between Ni, Mo, O, and Al. The intensity of the FTIR peaks for Ni-O, Mo-O and Al-O is related to the presence of these bonds. Thicknesses of the film after deposition and post-annealing were determined with *in-situ* and *ex-situ* spectroscopic ellipsometry (SE).

From Figure 1, the initial analysis of the wafers showed that there were no significant losses in Ni-O and Ni-OH intensities. There is less than 5 % change in the Ni-O stretch bonds peak intensities between wavenumbers 580 – 610 cm<sup>-1</sup>. However, the Al-O peak has decreased after annealing at 250C, highlighted in grey. As critical analysis of the passivation properties is ongoing, the lifetime of the wafers is increased with the Al<sub>2</sub>O<sub>3</sub> film. The deposition precursor TMA contains a large volume of hydrogen, which is known to passivate surface defects through hydrogenation (Corbett *et al.*, 1988). The final results will be discussed in the upcoming paper.



**Figure 1. Fourier-transform infrared of  $\text{Al}_2\text{O}_3$  capped  $\text{NiO}_x$  before and after thermal annealing at 250 °C and 460 °C**

#### References

- Black, L. E. and Kessels, W. M. M. (Erwin. (2018) 'Investigation of crystalline silicon surface passivation by positively charged  $\text{PO}_x/\text{Al}_2\text{O}_3$  stacks', *Solar Energy Materials and Solar Cells*. Elsevier B.V., 185(May), pp. 385–391. doi: 10.1016/j.solmat.2018.05.007.
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