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Structure of Molybdenum Nitride Films as Hole-Selective Contacts of Crystal Silicon Solar Cells determined with X-ray Scattering

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Molybdenum Nitride (MoNx) films are investigated as hole-selective layer of crystal Si solar cells due to having a proper work function (5.62 eV) and high conductivity (2000 S/cm). The hole-selectivity so far is limited by the poor surface passivation, which is highly correlated to the interface structure between Si and MoNx. The open circuit voltage and fill factor of devices with thicker MoNx film (200 nm) are better than those of thinner MoNx films (20 nm), which demonstrates that thicker MoNx films induce a better surface passivation and lower contact resistance at the same time. Moreover, the performance is different from MoOx films. Thick MoOx film (>20 nm) will induce a decreased fill factor due to their poor conductivity. In this work, the interface structure change between MoNx and Si is determined with X-ray reflectivity (XRR) analysis to figure out the passivation origin of MoNx films with different thickness. The phase structures and domain size of MoNx films with different thicknesses, compositions and crystallinity are determined with grazing incidence wide and small angle X-ray scattering (GIWAXS and GISAXS) to give important guidance for improving the hole-selectivity of MoNx further.

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