## ALD Grown ZnMgO:Al on Si for Photovoltaic Applications: Effect of High Mg Alloying and Al Doping.

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Heterojunction solar cells based on ZnO/Si employed as an emitter and absorber, present a high interfacial defect density due to the ~40% lattice mismatch between the two materials. Despite that, it has been predicted by simulations that a potential theoretical efficiency of ~24% can be achieved if the conduction band gap misalignment ( $\Delta E_C$ ) between ZnO and Si is eliminated by Mg alloying [1]. Experimentally an increase in efficiency from ~4% to ~7% can be achieved by following this route [2]. However, it has been also found that further improvement in efficiency is hindered by the increase in resistivity of the ZnO based layer when the Mg content overcomes ~2-3 at.%. In the present work it is found that by keeping the Al content equal to ~2 at.% and by increasing the Mg content up to ~12 at.% into the ZnO layers, the films still exhibit excellent electrical properties: carrier concentration and mobility equal to  $\sim 2 \times 10^{20}$  cm<sup>-3</sup> and  $\sim 2$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> as displayed in Fig.1(a) (experimental point with x<sub>Mg</sub> content < 5 are without Al). A constant increase of the open circuit voltage of the test solar cells from ~0.34 V (without Al doping) to ~0.44 V as a consequence of the Mg and Al introduction is observed as shown in Fig.1(b). The realized test solar cells with the optimized Mg and Al content exhibit an open circuit voltage, short circuit current density, efficiency, and fill factor equal to ~0.42 V, ~30 mA cm<sup>-2</sup>, ~7.5%, and ~60%, respectively. A realized device and I-V curve under standard illumination are shown in Fig.1(c).



**Fig1** (a) Carrier concentration, mobility, and resistivity vs Mg content (b) Open circuit voltage ( $V_{OC}$ ) dependence on the Mg content (c) I-V curve under standard illumination of a test solar cell with Mg~12 at.%. (In (a) and (c) experimental data with  $x_{Mg} < 5$  are without Al).

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