Simulation of nanohole point contacts for perovskite solar cells with insulating passivation layers

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Localised contacting strategies are well-established in silicon solar cells passivated with insulating materials as a way to achieve both low interface recombination and efficient charge extraction. A similar approach can be applied to passivated interfaces in perovskite solar cells (PSCs) between the active layer and one or both of the charge transport layers, however, only a small number of experimental demonstrations have so far been reported[1]. Few, if any theoretical analyses have been conducted to identify the optimum geometry of localised contacts, or when this approach could be beneficial for PSCs.

In PSCs, numerous interface passivation materials, including inorganic, organic and low-dimensional materials have been extensively explored for passivating defects and reducing non-radiative recombination at the perovskite-CTL (charge transport layer) interfaces. Among the materials used to improve interfacial properties in PSCs, insulating passivation materials such as polymers and 2D materials have achieved the highest performance[2–6]. However, the insulating nature of such materials increases the internal series resistance of the cell. These resistive losses tend to decrease the fill factor of the cell, leading to power losses. Introducing conductive pathways through the passivation layer via the nanohole contact approach can reduce series resistance while maintaining effective passivation (Figure 1).

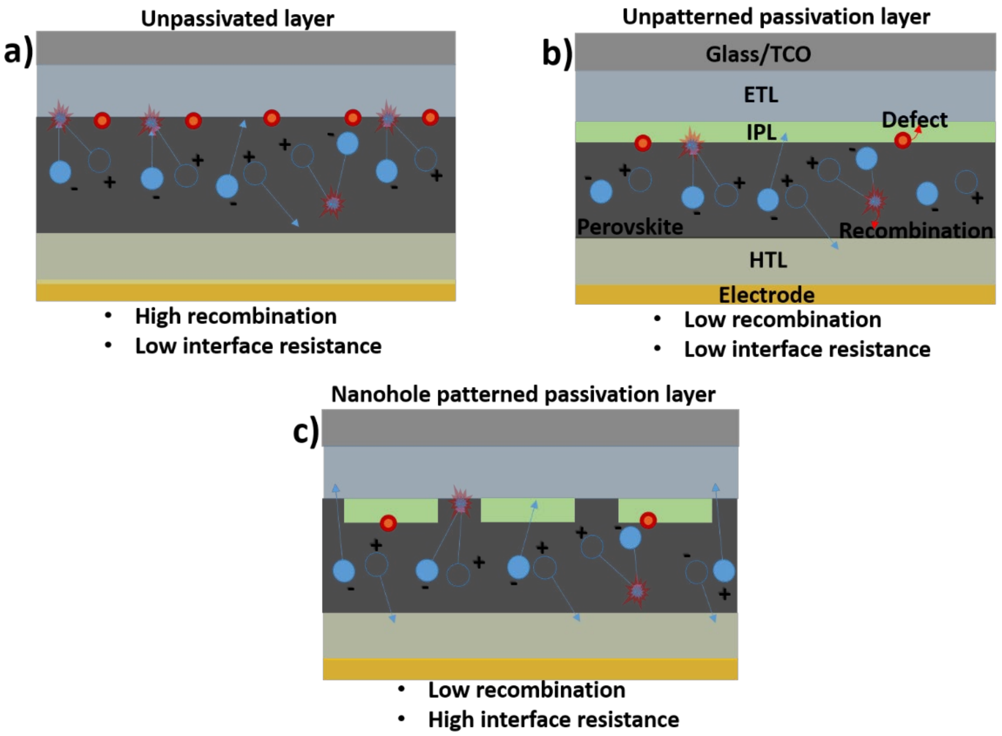

Figure 1. Schematic diagram of the device geometries without/with insulating passivation layer (IPL) (a) without IPL (planar), (b) with unpatterned IPL and (c) with nanohole patterned IPL, demonstrating their corresponding working mechanisms. Note that the arrow in (a-c) represents the flow of charges.

In this study, we investigate numerically, the potential for incorporating nanohole point contacts into insulating passivation layers at the perovskite-electron transport layer (ETL) interface as illustrated in Figure 1. We compare the modelled performance of planar (unpassivated) devices with devices that include a nanohole patterned passivation layer, for a range of defect densities at the unpassivated interface. For the modelled device parameters considered, we find that optimized nanopatterned passivation layer can provide a power conversion efficiency (PCE) gain of >5% absolute in the case of strong interface recombination, compared to an unpassivated cell. Efficiencies above 22% are predicted in optimized nanohole devices with surface defect densities as high as 2×10^{12} cm^{-2} compared to PCE~16% for the unpassivated reference device.

Figure 2. shows simulated PSC performance parameters plotted as a function of nanohole area fraction/spacing (pitch) and surface defect density of the unpassivated perovskite-ETL interface (in the nanoholes), for nanoholes of radius 50nm. The interface regions between the nanoholes are assumed to be perfectly passivated and insulating (no recombination and no charge transfer). Several key observations can be made from these contour plots: i) for any given defect density, increasing the pitch (reducing the area fraction of the nanoholes) increases the voltage due to improved passivation; ii) if the pitch is too large, the FF decreases rapidly due to the large distance that carriers must diffuse to be extracted via the nanoholes; iii) for any given defect density, there is an optimum nanohole pitch that maximises the PCE, and iv) the largest relative efficiency gains are achieved for higher interface defect densities.

Figure 3 compares the simulated performance of an unpassivated cell with that of an optimized nanohole-passivated cell for surface defect densities from 1.0×10^{11} cm^{-2} - 2.5×10^{12} cm^{-2}. At a low surface defect density of 1.0×10^{11} cm^{-2}, the PCE of both cells is maximum but for the unpassivated cell, PCE decreases sharply beyond 1.0×10^{12} cm^{-2}. In contrast, the passivated nanohole device retains much of its performance even at the highest defect density considered here. The PCE values extracted for the unpassivated cell are ~22.4% and ~13.6% for 1.0×10^{11} cm^{-2} and 2.5×10^{12} cm^{-2} surface defect density respectively. In contrast, the extracted PCE of the optimized passivated nanohole device only decreases slightly from ~23.1% to ~21.8%.

This study demonstrates nanohole point contacts have the potential to significantly improve the performance of PSCs that are limited by interface recombination. The nanohole concept opens up the possibility of using novel passivation layers such as TOPO[7], which has proven to offer outstanding defect passivation of perovskite films, but has not been successfully integrated into high efficiency cells because of its insulating properties. The simulations also provide guidance on the range of optimum feature sizes (pitch and hole size) and contact area coverage that would be required to apply this concept to typical perovskite devices.

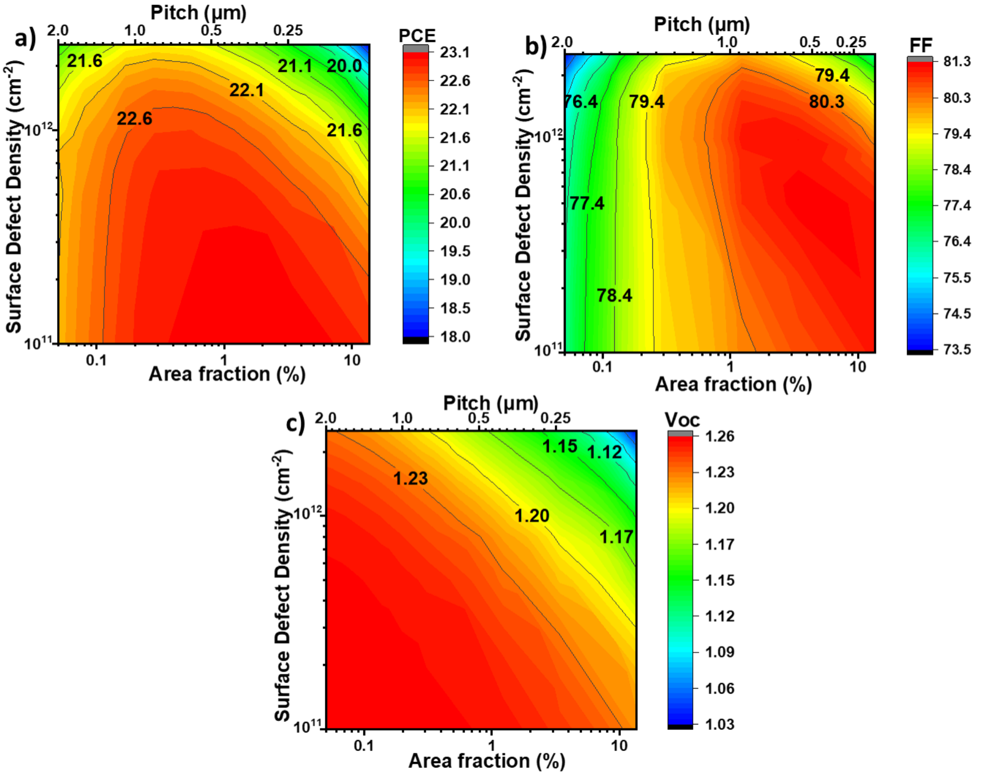

Figure 2. Photovoltaic parameters for surface defect density in the range of 1.0x10^{11} – 2.5x10^{12} cm^{-2} for (a) PCE (Power Conversion Efficiency) (b)Voc (Open-circuit voltage) and (c) FF (Fill Factor) at contact radius of 50 nm.

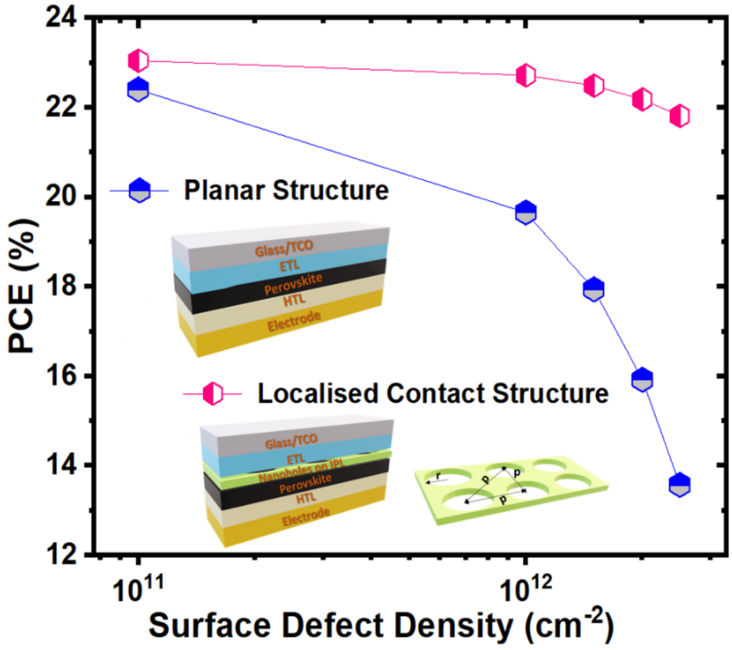

Figure 3. Power Conversion Efficiency (PCE) of planar and nanohole localised contact device strucures. The inset is the device structures of planar and nanohole localised contacts (and the unit cell of the IPL nanohole localised contacts, where p represents pitch and r represents contact radius of the hole size).

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