Monolithic 3-terminal perovskite/silicon HBT-based tandem compatible with industrial silicon bottom cells: a theoretical study

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Supplementary material: Details on TCAD device simulation

Figure 1 shows the *n-p-n* 3T-HBT device with a TIC configuration studied in the present work. From a computational point of view, simulating the full 2D geometry would imply a prohibitive mesh size, because of the unfavorable geometric aspect ratio between the physical dimensions in the horizontal direction, to take into account of the spacing between the metal contacts (which is typically on the mm scale), and the vertical direction (thickness of the stack layers, i.e. from micrometer down to tens of nanometers).

Thus, we have reduced the simulation domain to the quasi-1D one shown in Figure 2 (which we refer to as "intrinsic HBT" in the manuscript), where the T-emitter and R-collector are extended on the whole front and bottom surfaces, while the Z-base contact is placed laterally on the (n^+) -silicon layer.



Figure 1 Perovskite/Silicon 3T-HBTsc with TIC configuration Figure 2 Geometry for the quasi-1D simulation of the intrinsic HBT device

All the metal contacts are treated as ideal ohmic contacts in the drift-diffusion simulation and are considered as transparent in the optical simulation.

The quasi-1D device width (i.e., the distance between cutlines A and C) is small enough (micrometer scale) to not cause any loss associated to the lateral transport. This is seen by the energy band diagrams (Figure 3) taken at different cutlines: the quasi-Fermi levels are identical everywhere except for the mesh points where the ohmic base contact is placed (cutline C).



Figure 3 Energy band diagram at cutlines A and B in Fig. 2 (left) and at cutline C (right)

[1] Sentaurus Device, Synopsys Inc. (2017), http://www.synopsys.com.