

Interface-doping Effects and Gate-length Dependence of TMD/Metal Contacts

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Abstract

During the fabrication of 2D-material based MOSFETs, the metal electrodes undergo annealing, leading to a minor transition metal doping within the electrodes and resulting in interface doping. To simulate this scenario, we constructed two model structures: one with doping concentrated at the TMD/metal interface and the other with doping uniformly distributed throughout the metal electrode. Density Functional Theory (DFT) calculations on these models revealed that, unlike conventional silicon-based transistors, they are sensitive to gate length. Precise control of gate length to the sub-nanometer scale during fabrication can significantly impact their electrical properties.

Keywords - interface doping, gate length, DFT