Extraction of contact resistance from Green's function simulations of 2D material nanoribbon devices

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Promising electronic and transport properties of 2D material nanostructures are usually shrouded by contact resistance that limits their feasibility for high performance devices. In this work we extract contact resistance (R_C) from MOSFET simulations with silicene nanoribbons (SiNR) as channel material. We employ atomistic tight-binding Hamiltonians and top-of-barrier (ToB) MOSFET model combined with transmission and density of states (DOS) obtained from the device Green's function [1], [2]. Simulations are done for two cases: ideal contacts (ICs), where semi-infinite nanoribbons are assumed (Sancho-Rubio method), and metal contacts (MCs) defined within the wide-band limit (WBL) approximation with moderate interacting parameters and imaginary-only contact self-energy ($-\mathrm{Im}\Sigma^R_{S/D}$ = 1 eV) [3]. We assume that this model metal results in purely Ohmic contacts with SiNRs. The MCs are attached in the edge-contact geometry that enables encapsulation and preservation of 2D material properties (Fig. 1) [4]. The R_C is extracted from the difference in the ON-state current (I_{ON}) between the IC and MC case (Fig. 2). WBL metal contacts introduce Lorentzian peaks and oscillations into transmission (Fig. 3) and DOS (Fig. 4). The transmission is generally lower, which leads to decreased current driving capabilities of MC SiNR MOSFETs, whereas DOS exhibits similar averaged values and the appearance of metal-induced gap states (MIGS). The MIGS are localized on the atoms connected to MCs (not shown) so that states within the bandgap in Fig. 4 do not contribute to transport. When downscaling nanoribbon width (W) from 5.2 nm to 0.6 nm, I_{ON} decreases significantly for both types of contacts (Fig. 5). This behavior results in an increase of R_C from 196 Ωμm to 574 Ωμm when W is decreased from 5.2 nm to 0.6 nm (Fig. 6). The R_C value for silicene (limit of wide SiNRs) of ≈200 Ωμm agrees with experimental data for edge-contacted graphene (≈150 Ωμm [5]), which validates our approach despite the simplifications of the TB Hamiltonian and ToB device model.

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References: [1] A. Rahman et al., IEEE Trans. Electron Devices 50, 9, 1853–1864 (2003) [2] S. Kaneko et al., Appl. Phys. Express 7, 3, 035102 (2014) [3] M. Pourfath, The Non-Equilibrium Green's Function Method for Nanoscale Device Simulation, Springer-Verlag, 2014. [4] A. Jain et al., Nano Lett. 19, 10, 6914–6923 (2019) [5] L. Wang et al., Science 342, 6158, 614–617 (2013)

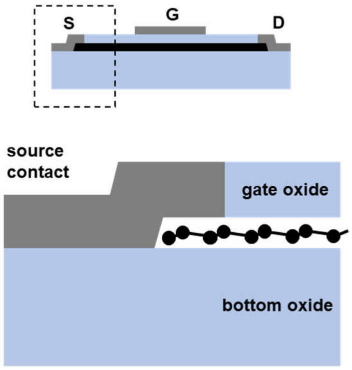

Fig.1: Illustration of a silicene nanoribbon MOSFET with S/D electrodes in edge-contact configuration.

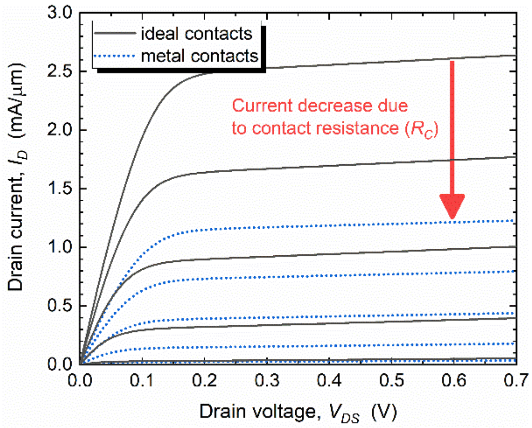

Fig.2: Output characteristics of SiNR MOSFETs with ideal and metal contacts. The SiNR channel is 4 nm wide and 15 nm long.

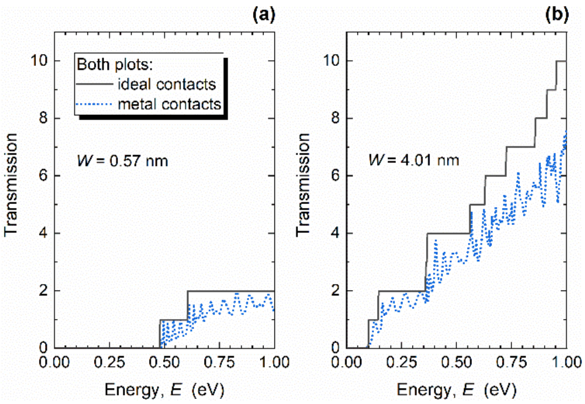

Fig.3: Transmission in (a) 0.57 nm and (b) 4.01 nm wide SiNRs with ideal and metal contacts.

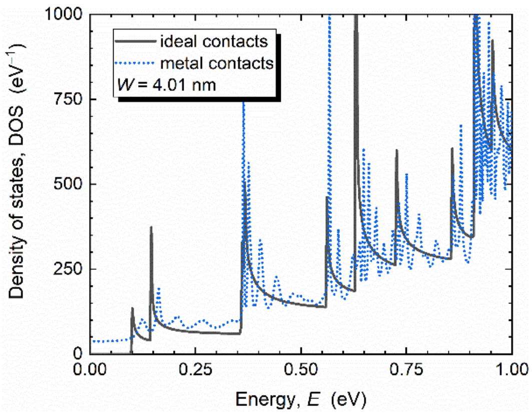

Fig.4: Density of states of 4.01 nm wide SiNRs with ideal and metal contacts.

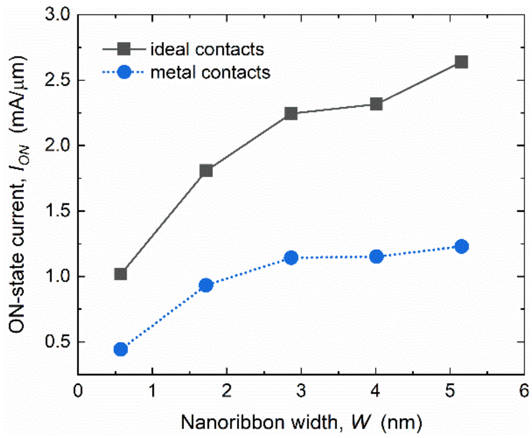

Fig.5: ON-state drain current vs. SiNR width in 15 nm long SiNR MOSFETs with ideal and metal contacts.

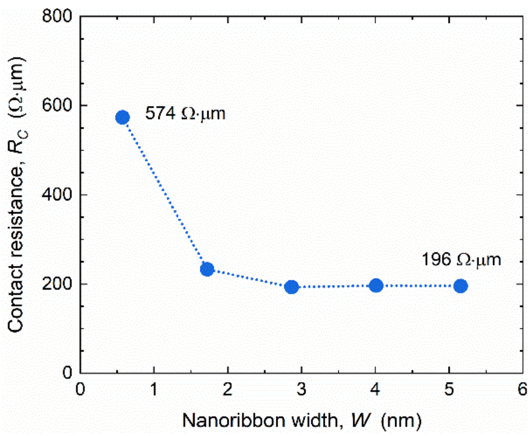

Fig.6: Impact of downscaling nanoribbon width on contact resistance in SiNR MOSFETs.

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