High-mobility InAs-AlSb core-shell nanowire heterostructures for thermoelectric energy conversion

G. B. Hirpessa*, S. Fust, R. Maier, F. Del Guidice, J. J. Finley and G. Koblmüller

Walter Schottky Institut and Physics Department, School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

*E-mail : Genetbacha.Hirpessa@tum.de

Thermoelectric energy conversion offers widespread applications in waste heat recovery for power generation and requires suitable materials with large thermoelectric conversion efficiency. To maximize figure-of-merit $ZT = \sigma S^2 T/\kappa$ relevant parameters such as electrical conductivity (σ), thermoelectric power factor (σS^2), and thermal conductivity (κ) need to be optimized for a given operating temperature T. Due to the interdependence between thermal and electrical properties, and Seebeck coefficient S, the optimization of parameters for high ZT is limited in bulk materials, but in nanostructures, the properties can be decoupled [1]. The aim of our work is to experimentally realize independent control of the Seebeck coefficient and electrical conductivity by exploiting the 1D density of states in very high mobility MBE grown III-V nanowires (NWs). First proof-of-principle studies demonstrating these effects were performed recently on modulation-doped GaAs-AlGaAs core-shell NWs, where enhanced σS^2, and strongly reduced κ were found [2]. While these initial studies were limited to low temperature, studying other III-V materials with lower electron effective mass is more appealing, in order to explore thermoelectric 1D-transport properties at higher temperatures with improved thermoelectric performance.

Here, we propose InAs-AlSb core-shell NW heterostructures as promising materials and show the first results on the growth using solid-source MBE on lithographically pre-patterned Si (111) substrates [3]. Creating high-mobility n-type (Si) modulated doped heterostructures is, however, particularly challenging in this system, since typical Si dopants are amphoteric and induce p-type behavior in AlSb. To mitigate this, two strategies are demonstrated: (i) Si-delta doping of a thin InAs QW embedded in the coaxial AlSb shell, and (ii) doping of a quaternary InAlAsSb shell lattice-matched to the InAs core (Figure 1). Correlated simulations of the band profiles and electron density distribution show clear formation of a high-mobility electron gas that is confined solely to the core InAs region when choosing InAs QW thickness of up to 5.5 nm and Si dopants (10^{19} cm^{-3}) placed in the center of the QW. For quaternary InAlAsSb with group-III and -V molar fractions in the mid-compositional range, Si δ-doping can be achieved directly in the shell without the need of an InAs QW (Figure 1). To realize InAs-QW based NW heterostructures, growth temperature optimization was necessary to induce highly symmetric growth of coaxial InAs QWs on the hexagonal NW sidewall facets, as found from cross-sectional He-ion microscopy. Likewise, we show the growth optimization routine for achieving InAlAsSb shell layers with composition tuned towards the mid-composition, and support these findings by STEM-EDX analysis (Figure 2). Finally, first examples of NW-field effect transistor (NWFET) test devices are shown, where both contact formation was established and gate-bias dependent electrical characterization was performed. 1-D sub-band quantization is found in InAs-AlSb core-shell NWs for temperatures up to 110K, which is about 40 K higher as in unpassivated InAs reference NWs (Figure 3), and much higher as in Si delta-doped GaAs-AlGaAs NWs.

[1] H. J. Goldsmid, Springer Series in Materials Science Vol. 121, pp 45-66 (2016)
[2] S. Fust, et al., Advanced Materials Vol. 32, No. 4 pp 1905458 (2020)
[3] F. del Giudice, et al., Applied Physics Letters Vol. 119 No. 19, pp 193102 (2021)
[4] G. B. Hirpessa, in preparation (2024).

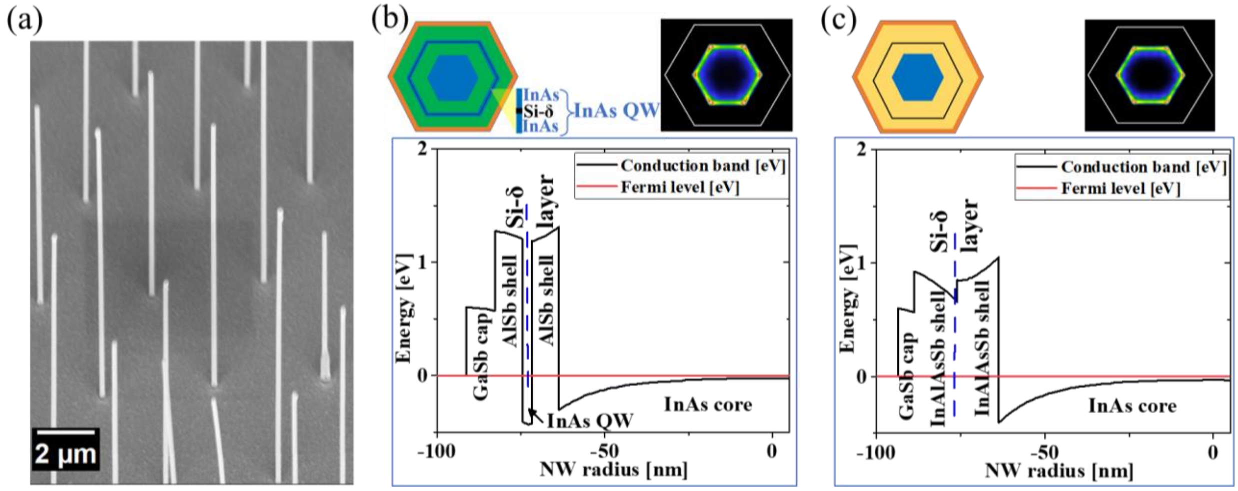

Fig. 1: MBE grown core-shell NWs and simulation data for different modulation doped structures; (a) InAs-AlSb core-shell NWs obtained by selective area epitaxy on prepatterned SiO_2/Si (111) substrate; (b,c) Schematic cross-section, band profiles, and corresponding electron density maps of (b) InAs-AlSb core-shell NW with InAs QW hosting a Si-δ layer, and (c) InAs-InAlAsSb core-shell NW with Si-δ doping layer at the center of the shell.

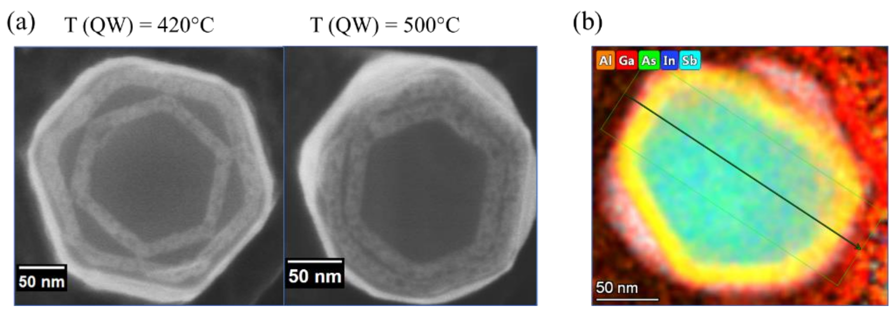

Fig. 2: (a) Helium ion microscopy (HIM) images of InAs-AlSb core-shell NWs with InAs QW embedded in the shell, for QW growth temperature of 420 °C (left, asymmetric growth) and 500 °C (right, symmetric growth); (b) STEM-EDX compositional map of the elemental distribution within an InAs-InAlAsSb core-shell NW.

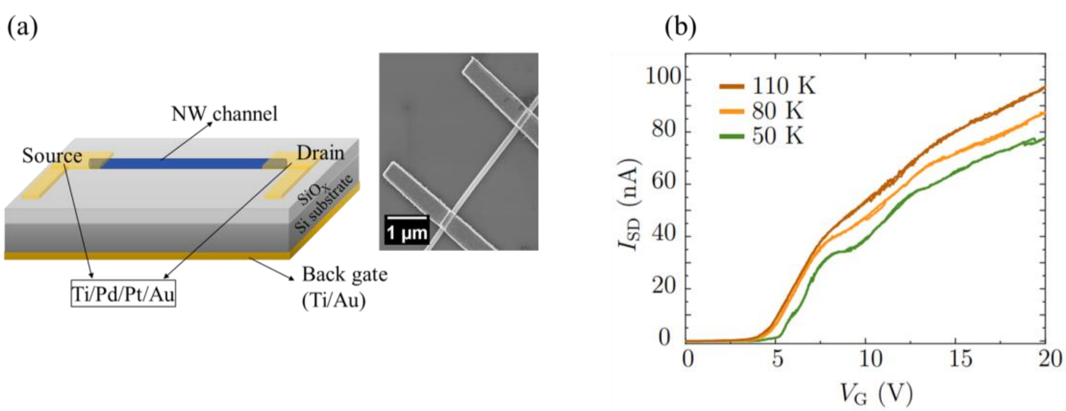

Fig. 3. (a) Schematic (left) and SEM image (right) of a NW field effect transistor (FET) with metallization profile used for InAs-AlSb core-shell NWs with GaSb cap; (b) temperature-dependent transfer characteristic of the NWFET at varying temperatures of 50 K, 80 K and 100 K.