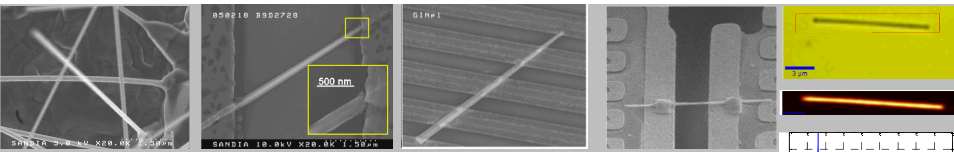
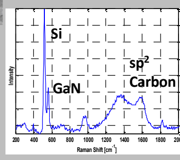
SAND2012-1322P

Sandia National Laboratories





Motivation: Uncontrolled resistance at metal contacts causes frequent device failure. From left to right, as grown ZnO nanowires, nanowire FET device with failure due to Joule heating at the contact interface, multiple embedded contacts to a single nanowire device, a thermoelectric device, and a high-efficiency light emitting device. The goal is to develop an understanding of electrical and thermal transport across contacts to nanostructures to yield improvement in performance and reliability. The question is: what creates variability in contact quality?

Devices: We determine structure, I-V curves and temperature maps in ZnO, GaN, and CNT in FET and mat-like configurations using Raman spectroscopy, thermal reflectance, and electron microscopy. We are able to ascertain electrical resistances, Schottky/Ohmic behavior, thermal conductivity and thermal contact resistance. Also, we are measuring the transient electron-phonon interaction processes. Taken together, these data inform device simulations and suggest the most important mechanisms controlling transport at the nanostructure-contact interface.

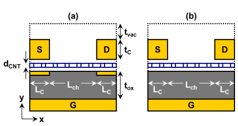
Contacts to Nanostructures

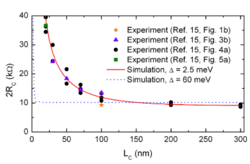
R. Jones (PI), F. Leonard, C. Spataru, T. Beechem, P. Yang, X. Zhou, P. Hopkins, D. Medlin, A. Cummings, and M. Shaughnessy

For nanoscale electronic, photovoltaic and sensing devices, the contact properties dominate the device performance. To realize the promise of nanotechnology, good engineering-level understanding of the contact physics is required. The approach is to use cutting-edge coupled experiments and theory, to determine what is required for contact modeling and which physical factors create good contacts.

We model the properties of carbon nanotube (CNT) field-effect transistors (FETs) using a Green's function technique that accounts for CNT-metal hybridization. This allows for a detailed study of the contact properties of ultra-small CNT FETs.

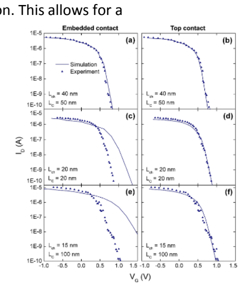
Device: CNT FET with embedded contacts (a) and with top contacts (b)





In order to fit the experimental contact resistance vs. contact length, we need a small value for the CNT-metal coupling strength.

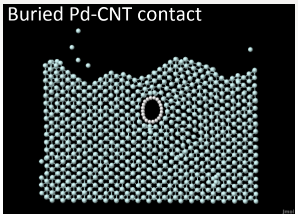
The coupling deduced from highly symmetrical first principles modeling is too large, suggesting the real device interface geometries are substantially different than idealized models.



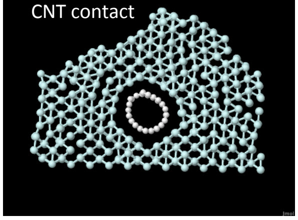
The good fit to the experimental subthreshold data suggests there is no contact metal below the CNT

How do annealing, contact composition and structural factors determine contact quality?

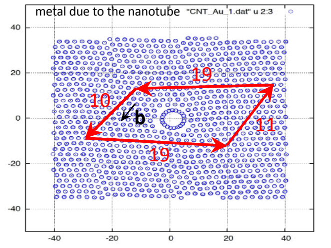
Buried Pd-CNT contact

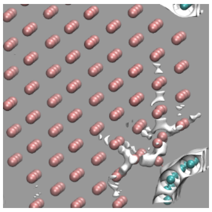


Buried Au-CNT contact



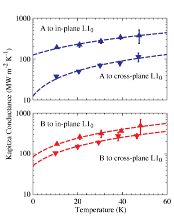
Post-Annealed Au-CNT contact, showing the formation of a dislocation in the metal due to the nanotube

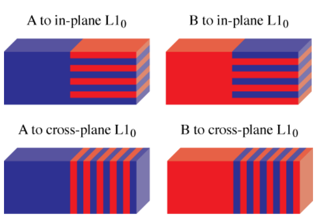




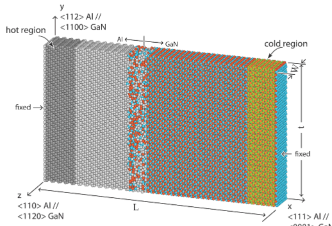
Electronic charge density isocontours at the CNT (turquoise)-metal (pink) interface, showing the effect of a nearby metal atom protrusion. The density of conduction states on the CNT and the coupling to the CNT depends sensitively on the metal atom locations

Phonon conductivity is correlated with structure and interface strength, much like the electronic conductivity. We investigate the structure-phonon transport relationship with idealized but realizable interface geometries.

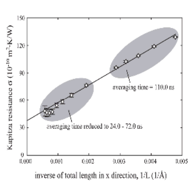


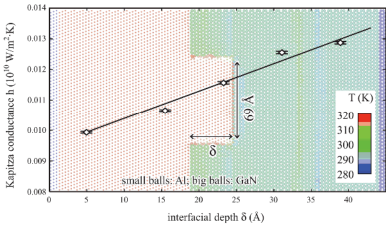


The presence of an interface can increase the anisotropy in thermal conductivity significantly beyond that inherent to the constituent materials. The thermal conductivity of the L1$_0$ AB alloy varies by a factor of two depending on orientation. The A to AB alloy interfaces (top), conductance varies by a factor of five depending on orientation, whereas for the B to AB alloy interfaces follows the trends in AB alloy thermal conductivity. We believe this is due to differing mismatch in the phonon DOS between the pure and the layered regions



In the figure, L = 14 Al + 28 GaN cells (98 Al + 146 GaN Å), t = 29 Al or 26 GaN cells (144 Å), W = 10 Al or 9 GaN cells (29 Å)





While rough interfaces generally give rise to increased thermal resistance, coherent structured interfaces and other "bridging" material can lower thermal resistance at the contact.

Next Steps: Given the understanding of the physics determining contact quality, the next step is to develop methods to control these factors during device fabrication. Process development and modeling can be based on optimizing the physical parameters we identify to increase performance and reliability.

U.S. DEPARTMENT OF ENERGY

NNSA

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
SAND No. 2011-XXXXP