ELECTRONIC AND ELECTRICAL PROPERTIES OF NANOSCALE INTERCONNECTS

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ABSTRACT

Interconnects deliver power and signals to transistors in computer chips and play an important role in modern electronics. Here we are focusing on the discovery and invention of new solutions that will enable both semiconductor and chemical industry to transcend known limits on interconnects. Based on density functional theory (DFT), We have explored the electronic structures of the interconnects made of a variety of carbon based materials. Then we have studied the chemical and physical properties for interconnect monolayers composed of short organic molecules. Our findings will open up opportunities for molecular level tailoring of a variety of interfacial properties for applications where nanolayers are not a viable option — such as in nano-devices or in thermally resistant molecular-inorganic hybrid devices.

Currently, copper wires are used as interconnects due to their superior electronic and electrical properties. As the interconnect line width decreases to nanoscale, electronic and electrical properties of copper get modified from their bulk values. These include, for example, high resistivity due to surface scattering and other properties such as finite number of channels near the Fermi level. It is important to explore these issues at a fundamental level, in addition to the search for additional materials so as to improve and prolong the use of the present electrical interconnects. It should be added here that many of these issues arise due to quantum confinement in the system and need to be studied using non-empirical techniques. While experiments continue to provide many important clues to enhance our understanding of these systems, computational and theoretical studies not only complement the experimental results but can also help decide the direction of future experiments.

Using first principles density functional method and Green's function based transport formalism we have studied electronic and electrical properties of systems ranging from copper nanowires to carbon nanotubes to graphene based systems. These computational studies were performed using massively parallel algorithms and supercomputers which has helped us to address many outstanding issues that were not possible otherwise. We were able to investigate at a fundamental level the

role of organic molecules in improving mechanical properties of copper-dielectric interfaces important for the near term use of copper as interconnect material. Our first principles based calculation results suggest that electrical properties of copper wires get drastically modified below 10nm due to quantum confinement. At these length scales metallic single-walled carbon nanotube bundles were found to outperform copper based interconnects.

Graphene nanoribbons (GNRs) due to their planar nature have attracted much attention for potential applications as future electrical interconnects. In particular, just like CNTs GNRs have long electron mean free path ($\sim \mu$m), high carrier mobility ($10^5 cm^2/V \cdot s$), excellent mechanical strength (tensile strength $\sim$ 100GPa) and high thermal conductivities ($300\, W/m \cdot K$), and have shown great promise for integration with existing CMOS technology. The current carrying capacity of both CNT and GNR are remarkable ($> 10^{10} A/cm^2$), which is about 4 orders of magnitude higher than copper even at $\sim$ 1nm diameter. Under the current technology, GNR can be produced using lithography techniques down to tens of nanometers.

In spite of these promises many challenges still remain before either of these new solutions become viable. These problems arise mainly due to size-effects at such diminished length scales. Quantum effects such as discrete energy levels, modified electron-phonon coupling become severe at nanoscale and these issues appear (or will appear) in all the emerging interconnects e.g. CNT, GNR, single crystal metallic wires (atomic wires) including copper at nanoscale. Both theoretical and experimental studies are beginning to provide answers to some of these questions related to carrier transport at nanoscale, otherwise known as "quantum transport", but much work is still needed in this direction. Using large scale quantum simulations we have addressed a few of these issues. These include: (1) effect of different dielectrics, including low-k materials, on wire's electrical properties (e.g. RC delay etc.) (2) stability and bonding of the wires with the underlying substrate (3) variation in the electronic properties of stacked graphenes with the number of layers (4) mechanical properties of carbon based interconnects (5) comparison of electronic and electrical properties of Ag and Cu wires at nanoscale. In addition, we have studied edge-functionalized GNRs which provide a new and interesting approach to

enhance their electrical performance. These systems are a new class of materials that may provide superior performance and could integrate into existing CMOS technology better. We have made comparisons with available experimental data whenever possible and believe that our results can provide valuable inputs for compact and circuit level simulations.