For high performance computer design a search for new materials and their modeling is required as current semiconductor technology is approaching to its limit.

Using state of the art density functional theory (DFT) we have modeled carbon based emerging VLSI interconnects. We used high-performance computers (HPC) hosted in LSU to calculate electronic transport properties, and vibrational properties of graphene based VLSI interconnect. A non-linear iterative numerical approach has been proposed for electro-thermal transport coupling to incorporate electronic scattering due to phonon.

We have considered following materials in this study.
2. Graphene Nanoribbon on Copper.

Analytic:
For the modeling of CNT we have developed an iterative self consistent analytic model for solving electro-thermal coupled equation. (Fig. 3.)

First Principle Method (DFT):
For Graphene/Copper nanoribbon there is no existing model. So we modeled it for the first time using First principle Method and DFT calculations using HPC resources. (Fig. 7.)

Method shown in Fig. 3 can be used to,
1. Estimate maximum bias voltage a CNT interconnect will withstand.
2. Explain breakdown phenomena.
3. Hot spot detection.
4. Explaining experiments where heat is a concern.

Computational framework shown Fig. 7, is useful to estimate electrical properties of any emerging interconnect materials. Few key results,
1. Graphene/Copper (G/Cu) is better in terms of electrical and thermal conductivity.
2. G/Cu has more DOS near Fermi energy to be more conductive.
3. G/Cu provides more thermal dissipation pathway than Cu or Graphene only interconnect.
4. Compatible with CMOS and good candidate for 5nm node.

As an alternative to existing Cu-low-k interconnect, carbon based materials are studied. An analytic model is proposed to study CNT interconnect with Joule heating [1].

G/Cu nanoribbon is proposed as more auspicious interconnect material with evidence from First principle study [2-3]. More hybrid 2D, 1D metallic system need to be explored. For circuit simulation analytic model need to be developed.

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References