Contact resistance in metal/graphene junctions from first principles

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Edge metal-graphene (Me-G) contacts have been shown experimentally to achieve contact resistances with similar or lower values than most top contacts [4], challenging the conventional wisdom and some experimental results that having a large contact area will result in a decreased value of the contact resistance. Attempts at explaining this behavior resort to the perceived need of electrons to scatter from a value with $k_z \neq 0$ to $k_z=0$ when entering the graphene layer.
Based on first-principles calculations, we find that ballistic electron injection into graphene (or any other 2D material) is a perimeter-dependent phenomenon, dependent only on the atomistic details of the graphene-metal configuration at the edge of the metal.
We study an Al/Graphene flake contact, showing a square root dependence of the transmitted current with the contact area, and graphene with a varying overlap on top of a Me(111) surface (Me=Ni, Al, Pd, graphite), showing that a large fraction of the theoretical maximum of the conductance per unit width is achieved even with a very small overlapping region between graphene and the Me(111) surface (Fig. 1), with values similar to the edge contact.
From these results it can be concluded that the experimentally observed high contact resistances in metal – 2D material junctions may be amendable if proper care is taken that the edge region has an intimate contact with the metal. In fact, having a large overlapping region between the metal and the 2D material may be detrimental to the goal of a low contact resistance.
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References

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Figures

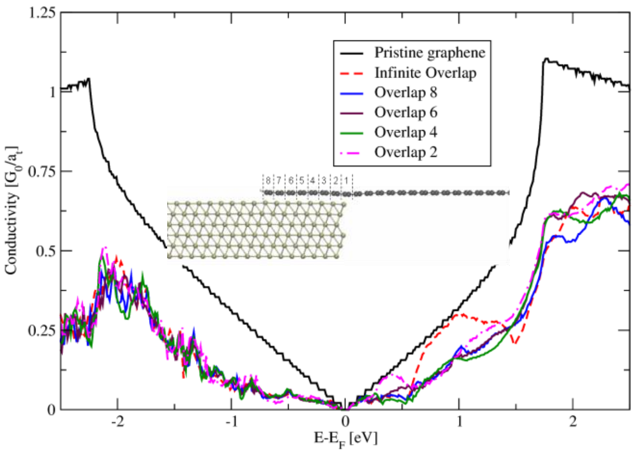

Figure 1: Minority spin line conductivity for a relaxed G/Ni(111) structure with varying amount of overlap (inset).