Atomic-scale model for the contact resistance of the nickel-graphene interface

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Motivation and overview

- **Purpose:** Understand contact resistance between graphene and metals
- **Device-like** geometries
- Study different edge geometries
- Covalently bonded (chemisorbed) graphene on Ni surfaces
  - ~1% lattice mismatch between Ni (111) and graphene

\[ V_b = -0.1 \, V \]
Optimized system geometries

Ni (111) – zigzag, 4 Å overlap

Ni (111) – zigzag, 8 Å overlap

Ni (111) – zigzag, 4 Å overlap, H-termination

Ni (100) – armchair, 8 Å overlap, H-termination
Computational details

- **Code:** Atomistix ToolKit
- **DFT**
  - LSDA (Perdew-Zunger)
  - DZP basis set (SIESTA-type)
    - 15 orbitals per Ni atom, 13 per C
    - 9 k-points in the infinite graphene sheet direction
  - Extended basis set range for proper work function
- **Non-equilibrium Green’s function (NEGF) method to compute transport properties**
  - FFT in XY, multigrid/Dirichlet in Z (transport direction)
NEGF transport methodology

Electronic structure
- DFT, Extended Hückel, TB, ...

Transport
- Exact description of semi-infinite electrodes via self-energies
- Non-equilibrium electron distribution using NEGF

Electron current (Landauer formalism)

Transmission spectra

• Summed over spin
• 501 k-points in B
• Similar low-bias slope for all systems: $0.06 \, \text{G}_0/(\text{eV}\,\text{Å})$
• Ideal graphene sheet: $0.12 \, \text{G}_0/(\text{eV}\,\text{Å})$
Transmission coefficients

\( E - E_f = 0.05 \text{ eV} \)

Note: System (b) has larger overlap (8 Å) than (a) (4 Å)
System (b) @ $E - E_f = 0.05$ eV. Current incident from the right.

Current density drops at surface - overlap region is not important for contact resistance.
Charge transfer

For non-terminated graphene: electron accumulation at the edge

Electrostatic potential inside the graphene sheet

Net Mulliken charges; per atom (bars) and accumulated from the far-right (red line)

For H-terminated graphene: electron depletion at the edge

In all cases: electron transfer from graphene to Ni (red curve, C>15 Å)
The system can be divided into two parts:
- (MG) the metal surface with the bonded graphene atoms
- (G) the non-bonded graphene
Contact resistance model (2)

- Diagonalize (MG) into left- and right-going modes.
- An incoming left-going electron from (G) may couple with either the left- or right-going modes in system (MG).
- In the strong coupling regime, the carbon atoms in (MG) will be enough perturbed by the metal surface that neither left- nor right-going modes bear any resemblance to the modes in (G).
- Thus, incoming electrons from (G) will have roughly the same coupling strength with left- and right-going modes in (MG), and thus approximately half of the incoming current is transmitted through the system (and half is reflected).
- In conclusion, the contact resistance is **twice the ideal value**, independently of contact area and other contact details.
Non-self-consistent extended Hückel model
Graphene on Al

$E - E_f = 0.05 \text{ eV}$

Finally: compute the contact resistance

\[ \frac{1}{R} = G_0 \times 0.06 \text{ (eVÅ)}^{-1} \int E \frac{\partial f}{\partial E} dE \]

\[ R \approx 600 \text{ Ωµm} \]

Cf. experimental data: 800 Ωµm also independent of contact area
[K. Nagashio et al., APL 97, 143514 (2010)]
Summary

- The contact resistance between Ni and graphene is independent of the contact area and direction of the graphene sheet.
- The value is ~600 Ωµm = 2x the ideal quantum contact resistance.
- Both observations are in excellent agreement with experimental data.
- Model calculations predict that this result is generic for strongly bonded graphene on metal surfaces (Co, Pd, Ni, Ti).