Magnetoresistance and negative differential resistance in Ni|Graphene|Ni junctions driven by finite bias voltage: A first-principles study

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One of the great successes of first-principles quantum transport modeling has been a conjecture [1] of *very large* "optimistic" tunneling magnetoresistance, $\mathrm{TMR} = (G_\mathrm{P} - G_\mathrm{AP})/G_\mathrm{AP} \times 100\% \geq 1000\%$, in Fe|MgO|Fe(100) MTJs where G_P (G_AP) is conductance for parallel (antiparallel) orientation of the Fe magnetizations. This prediction has ignited intense fabrication efforts reaching TMR of about 200% at room temperature which, although undoubtedly correlated with the crystallinity of MgO barrier, is difficult to reconcile with first-principles results [1]. The origin of the discrepancy is the sensitivity of spin injection and TMR to details of difficult-to-control interfacial disorder as revealed by a number of theoretically investigated scenarios (such as the intermixing of Fe and MgO, oxygen vacancies at or near the Fe|MgO interface, or substoichiometric FeO layers with small oxygen concentrations). In addition, TMR in MgO-based MTJs decays precipitously with increasing bias voltage where the specific features of the decay are also sensitive to the type of interfacial disorder.

These issues could be resolved by searching for new material systems which would ensure perfect spin filtering [2] in the absence of disorder while being much less sensitive to the presence of interfacial disorder in realistic junctions. The Ni|Gr_n|Ni junctions—where n layers of graphene (Gr_n) are sandwiched between two Ni electrodes as illustrated in Fig. 1—exploit the very small mismatch of 1.3% between the in-plane lattice constant of Gr and surface lattice constant of Ni, as well as the fact that majority spin states of Ni are absent in a large region around the K point, to achieve perfect spin filtering for $n \geq 5$, as quantified by the "pessimistic" magnetoresistance $\mathrm{MR} = (G_\mathrm{P} - G_\mathrm{AP})/G_\mathrm{P} \times 100\% \approx 100$ % (the "optimistic" MR diverges since G_AP vanishes for large n).

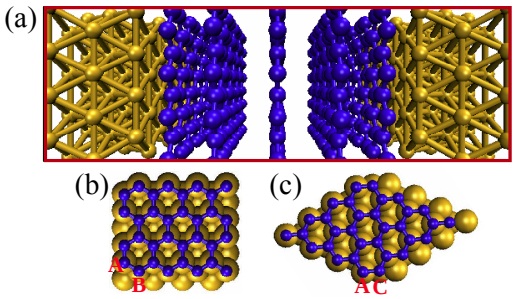

Fig. 1. (Color online) (a) Schematic view of Ni|Gr_5|Ni junction where Gr_5 represents five layers of graphene and Ni is (111) fcc nickel. The device extends to infinity along the transverse directions while Ni electrode (orange) are semi-infinite in the longitudinal (transport) direction. The two investigated types of bonding for Gr on the Ni(111) surface are illustrated in panel (b), as AB configuration where the two carbon atoms in the graphene unit cell cover Ni atoms in layers A (surface) and B (second layer), and panel (c) as AC configuration in which carbon atoms are placed directly above the Ni atoms in layers A (surface) and C (third layer). Here ABC refers to three close-packed layers within an fcc crystal.

We employ spin- and k-resolved nonequilibrium Green function formalism combined with density functional theory to study finite-bias quantum transport in Ni|Gr_n|Ni perpendicular junctions where n graphene layers are sandwiched between two semi-infinite Ni(111) electrodes. We find that recently predicted "pessimistic" magnetoresistance of

100% for $n \geq 5$ junctions at zero bias voltage $V_b \to 0$, persists up to $V_b \simeq 0.4$ V which makes these junctions promising for spin-transfer-torque-based device applications. In addition, for parallel orientations of the Ni magnetizations, the $n = 5$ junction exhibits a pronounced negative differential resistance as the bias voltage is increased from $V_b = 0$ V to $V_b \simeq 0.5$ V. We confirm that both of these nonequilibrium effects hold for different types of bonding of Gr on the Ni(111) surface while maintaining Bernal stacking between individual Gr layers.

Our principal results are shown in Figs. 2 and 3. Fig. 2(a) shows the zero bias "pessimistic" MR reaching 100% for barriers composed of $n \geq 5$ graphene layers and Fig. 2(b) predicts that such maximized MR would persist even at finite $V_b \simeq 0.4$ V. Figure 2(b) also suggests that bias voltage dependence of MR can be employed experimentally to determine the type of bonding configuration for Gr on the Ni(111) surface. Furthermore, Fig. 3 shows that Ni|Gr$_n$|Ni junction with P orientation of the Ni magnetizations will exhibit pronounced negative differential resistance (NDR), where total charge current first increases and then decreases as the bias voltage is increased from $V_b = 0$ V to $V_b \simeq 0.5$ V (or symmetrically in the opposite direction).

References

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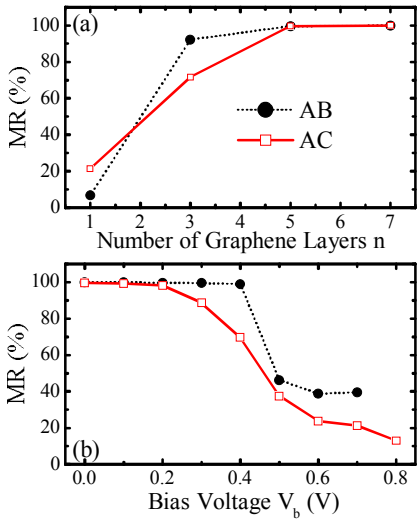

Fig. 2. (Color online) (a) The "pessimistic" TMR for Ni|Gr$_n$|Ni junctions as a function of the number of graphene layers n and for two different, AB and AC, bonding configurations for Gr on the Ni(111) surface illustrated in Fig. 1(b) and (c), respectively. (b) The "pessimistic" TMR for $n = 5$ junction versus finite bias voltage for AC and AB bonding configurations.

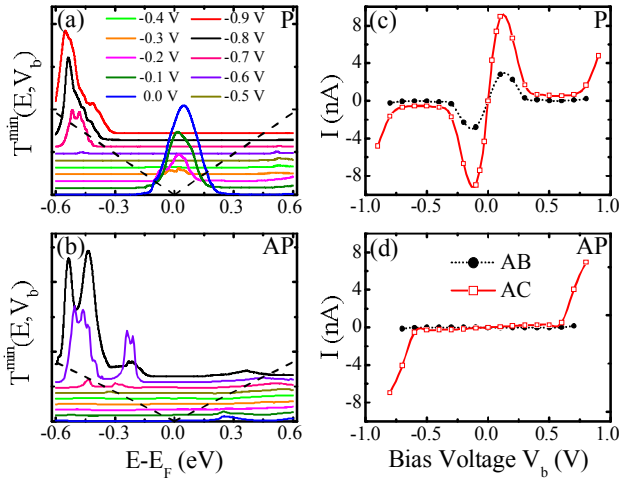

Fig. 3. (Color online) The finite-bias transmission function $T^{\min}(E, V_b)$ for Ni|Gr$_n$|Ni junction in AC bonding configuration at the Ni(111)|Gr interface [Fig. 1(c)] for (a) P and (b) AP orientations of the Ni magnetizations. Since in P orientation minority spin contribution dominates, while in AP setup both minority and majority spins contribute the same, only $T^{\min}(E, V_b)$ is presented here for both P and AP orientations with curves at different V_b shifted along the y-axis for clarity. Panels (c) and (d) show *I-V* characteristics for P and AP orientation, respectively. The NDR is conspicuous in P orientation in panel (c) for both AC and AB bonding configuration.