Landauer formalism modeling for <u>total</u> thermionic current in reverse-biased Ideal Graphene/n-Si Schottky junctions

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The typical current-voltage relationship predicted by basic thermionic emission modeling, namely, $j = A^*T^2 \exp(-q\Phi_b/kT)\,[\exp(qV/kT)-1]$, ($q\Phi_b$ the junction barrier, V the applied voltage, and A* Richardson's constant) does not include specific carrier transport mechanisms that occur across the graphene/semiconductor Schottky junction (G/n-Si junction). In a reverse biased G/n-Si junction, graphene's fermi level shifts upwards relative to the semiconductor's fermi level, through the reversely applied voltage though the junction. Reverse current (G to Si side) is probable via thermionic escape. In this communication we propose a way of re-writing, from first principles, the formula for thermionic carrier transport across an ideal Schottky G/n-Si junction under reverse bias, by considering two groups of migrating carriers: those carriers that surmount over and tunnel through the junction barrier spike $q\Phi_b$. We model carrier escape in a Landauer scheme, by expressing the current over or through the Schottky junction spike, namely, $J = (q/t_g)\int dE \times D(E) \times (f_g - f_S) \times f(E) \times v(E) \times t(E)$, where q is the electronic charge, t_g is the thickness of the graphene layer D(E) is graphene's linear DOS (density of states), $f_{g,S}$ are the Fermi-Dirac carrier probability functions, v(E) is the thermal electron velocity, and t(E) is the transmission probability over (=1) and through (less than 1) the barrier. Starting from the last integral, we model migrating carriers through two transport mechanisms (a) thermionic escape (TE) over the junction barrier and (b) thermionic field emission (TFE) through the barrier. In the first case, electrons are modeled as carriers surmounting the junction barrier with maximum probability ($|t| = 1$), and in the latter, carriers are modeled as tunneling through the junction barrier with a non-zero probability $|t| = \exp(-q\Phi_b/E_{oo})$. The denominator in the probability exponential depends on semiconductor donor doping N_d according to $E_{oo} = (q\hbar/2)\sqrt{N_d}/\sqrt{m^*\varepsilon_s}$, where m* is the semiconductor's effective mass and ε_s is its dielectric constant. We calculate both TE and TFE currents explicitly: (1) TE current is explicitly derived as $J_{TE} = A_1^*\, T^{1.5} \exp(-q\Phi_b/kT)\,[1-\exp(-qV/kT)]$ and (2) TFE current: $J_{TFE} = A_2^*\, T^{2.5} \exp(-q\Phi_b/\mathbf{n}kT)\,[1-\exp(-qV/kT)]$, where **n** is the junction *quality factor* directly dependent on the tunneling probability |t| through the potential spike at the junction at energy values under $q\Phi_b$; the parameter n can be found explicitly as $n = \gamma N_d^{1/2}$, with γ an appropriate constant ($\gamma \sim 10^{-12} m^{3/2}$) related to carrier effective mass, semiconductor dielectric constant and the kT parameter. For total current, we the sum of TE and TFE components will suffice: $J = [A_1^*T^{3/2} \exp(-q\Phi_b/kT) + A_2^*T^{5/2} \exp(-q\Phi_b/nkT)]\,(1-\exp(-qV/kT))$. We see from this last result, that temperature dependence is smeared between concurrent $T^{1.5}$ and $T^{2.5}$ dependences respectively, and two new Richardson-like constants A_1^*, and A_2^*, containing the thickness of the 2-D graphene layer; different Richardson's constants appear because of the graphene layer replacing the metal of a traditional Schottky junction. The quality factor n in the second exponential is related to the semiconductor's donor doping level as $N_d^{1/2}$; with values expected to be between 0.10 and 0.316 for semiconductor doping levels from $N_d = 10^{16}$ to 10^{17} cm^{-3} respectively. Alternatively, the total current can also be written in a more general form: $J = A_1^*T^{3/2} \exp(-q\Phi_b/kT)\,[1 + (3/2)(kT/q\Phi_b) \exp(-q\Phi_b/mkT)]\,(1-\exp(-qV/kT))$; with $kT \ll q\Phi_b$, and m a new version of the original factor $m = n/(n-1)$.