

## Combined thermionic emission and tunneling currents model for Graphene/n-Si Schottky Barriers under reverse bias

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Fundamental understanding of carrier transport is needed for current graphene-based devices (e.g. graphene based FET's or G-FET's, solar cells) involving a single G-layers grown over n- or p- type semiconductors (e.g. Si). Carriers overcome potential barriers in Schottky contacts or barriers (SB) in two ways (a) by thermionic emission and (b) by field emission mechanisms. In all, a combined theory of these mechanisms is eventually needed for a better understanding of electron/hole transport. In this paper we deal with one of these two aspects of electron transport from graphene to n-type semiconductor, namely, thermionic emission. Our new modeling considers incident carriers from the graphene side, with sufficient energy to overcome a G/n-semiconductor SB contact potential, and includes a single graphene layer in direct contact with n-type semiconductor, leading to a first-principles calculation of thermionic current under reverse bias for the first time. Specifically, for a junction between a single graphene layer and an n-type semiconductor (n-Si), we predict thermionic emission current directly related to (a) temperature (b) applied bias (c) junction barrier and (d) graphene layer thickness  $t_g$ . We find a  $T^{3/2}$  -temperature dependence (instead of a  $T^2$ -dependence of common metal-semiconductor SB's). The predicted current from graphene to the semiconductor is  $J = A^* T^{3/2} \exp(-q\Phi_B/kT) \exp((qV/kT) - 1)$ ; Where  $A^*$  is a new Richardson's constant ( $A/m^2/^\circ K^{3/2}$ ),  $q\Phi_B$  is the potential barrier at the G/n-Si contact relative to the graphene layer's Fermi level,  $V$  is the reverse applied voltage. Our result is attributed to graphene's density of states (DOS) linear dependence on energy ( $D(E) = D_0 E$ ), and resembles similar temp-dependence of thermionic currents in 2-dimensional structures (thermal escape over the barrier of quantum wells in GaAs/AlGaAs multi-quantum wells and superlattices) and agrees with the common thermionic emission of regular metal-semiconductor contacts. Probing further, we propose a new model for tunneling and field emission current in G/n-Si junctions, based on the Landauer formalism. We derive a  $T^2$ -dependent explicit result for tunneling current:  $J = A^{**} T^2 |t| \exp(-q\Phi_B/kT) \exp((qV/kT) - 1)$ , where  $A^{**}$  is an explicitly derived Richardson-like constant for tunneling processes,  $|t|$  is the tunneling probability directly related (and shown) to the contact barrier  $q\Phi_B$ . By combined both processes, we propose a new model for total current  $J$  as the sum of thermionic and tunneling currents:  $J = (A^* T^{3/2} + A^{**} T^2) \exp(-q\Phi_B/kT) \exp((qV/kT) - 1)$ .